



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:17 PM UTC

PDB ID : 5YKG / pdb_00005ykg
EMDB ID : EMD-6833
Title : Structure of pancreatic ATP-sensitive potassium channel bound with glibenclamide and ATPgammaS (Class2 at 4.57Å)
Authors : Chen, L.; Wu, J.X.
Deposited on : 2017-10-14
Resolution : 4.57 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

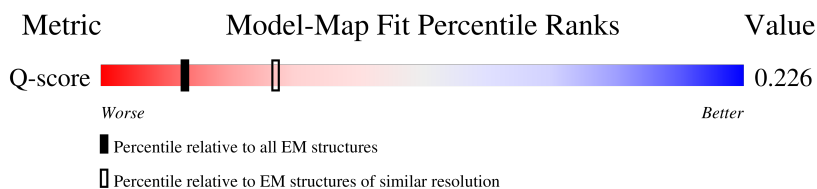
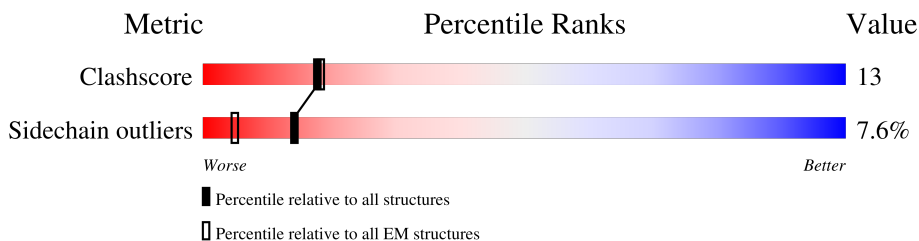
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.57 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2418 (4.07 - 5.07)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	390	
1	C	390	
1	E	390	
1	G	390	
2	B	1582	

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Mol	Chain	Length	Quality of chain
2	D	1582	13% 59% 22% • 17%
2	F	1582	13% 59% 22% • 17%
2	H	1582	13% 61% 22% • 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 50868 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

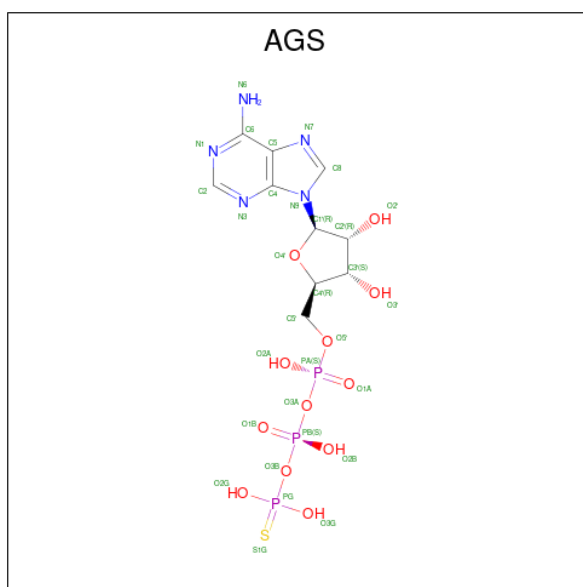
- Molecule 1 is a protein called ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	325	Total	C	N	O	S	0	0
			2433	1574	415	429	15		
1	C	325	Total	C	N	O	S	0	0
			2433	1574	415	429	15		
1	E	325	Total	C	N	O	S	0	0
			2433	1574	415	429	15		
1	G	325	Total	C	N	O	S	0	0
			2433	1574	415	429	15		

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8 isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1309	Total	C	N	O	S	0	0
			10189	6644	1724	1768	53		
2	D	1309	Total	C	N	O	S	0	0
			10189	6644	1724	1768	53		
2	F	1309	Total	C	N	O	S	0	0
			10189	6644	1724	1768	53		
2	H	1309	Total	C	N	O	S	0	0
			10189	6644	1724	1768	53		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms					AltConf	
3	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	E	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	G	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	H	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

- Molecule 4 is 5-chloro-N-(2-{4-[(cyclohexylcarbamoyl)sulfamoyl]phenyl}ethyl)-2-methoxybenzamide (CCD ID: GBM) (formula: C₂₃H₂₈ClN₃O₅S).

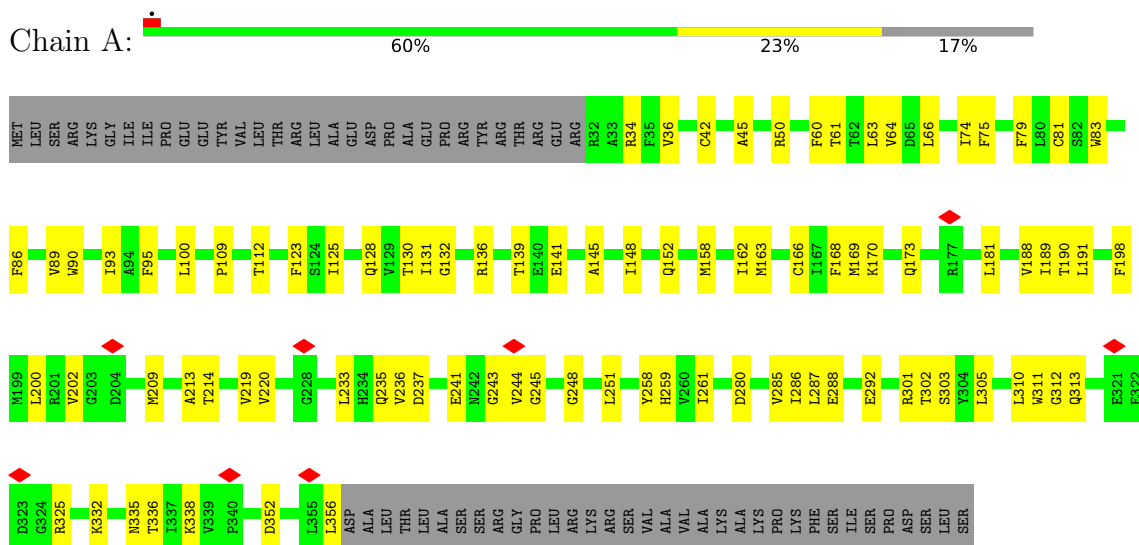


Mol	Chain	Residues	Atoms						AltConf
4	B	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0
4	D	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0
4	F	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0
4	H	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0

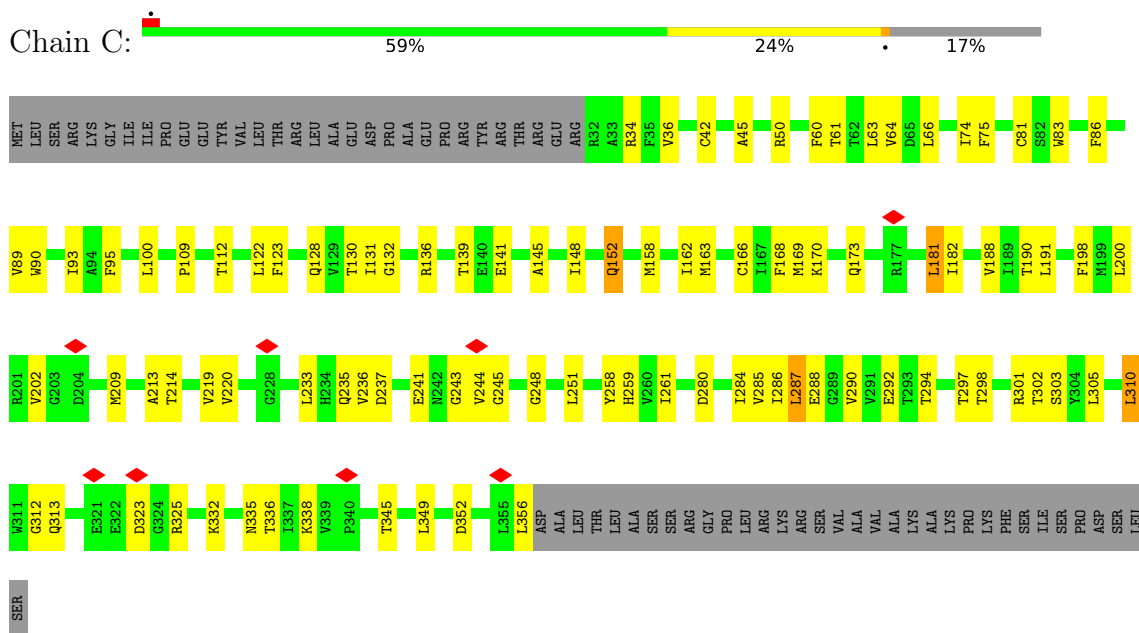
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



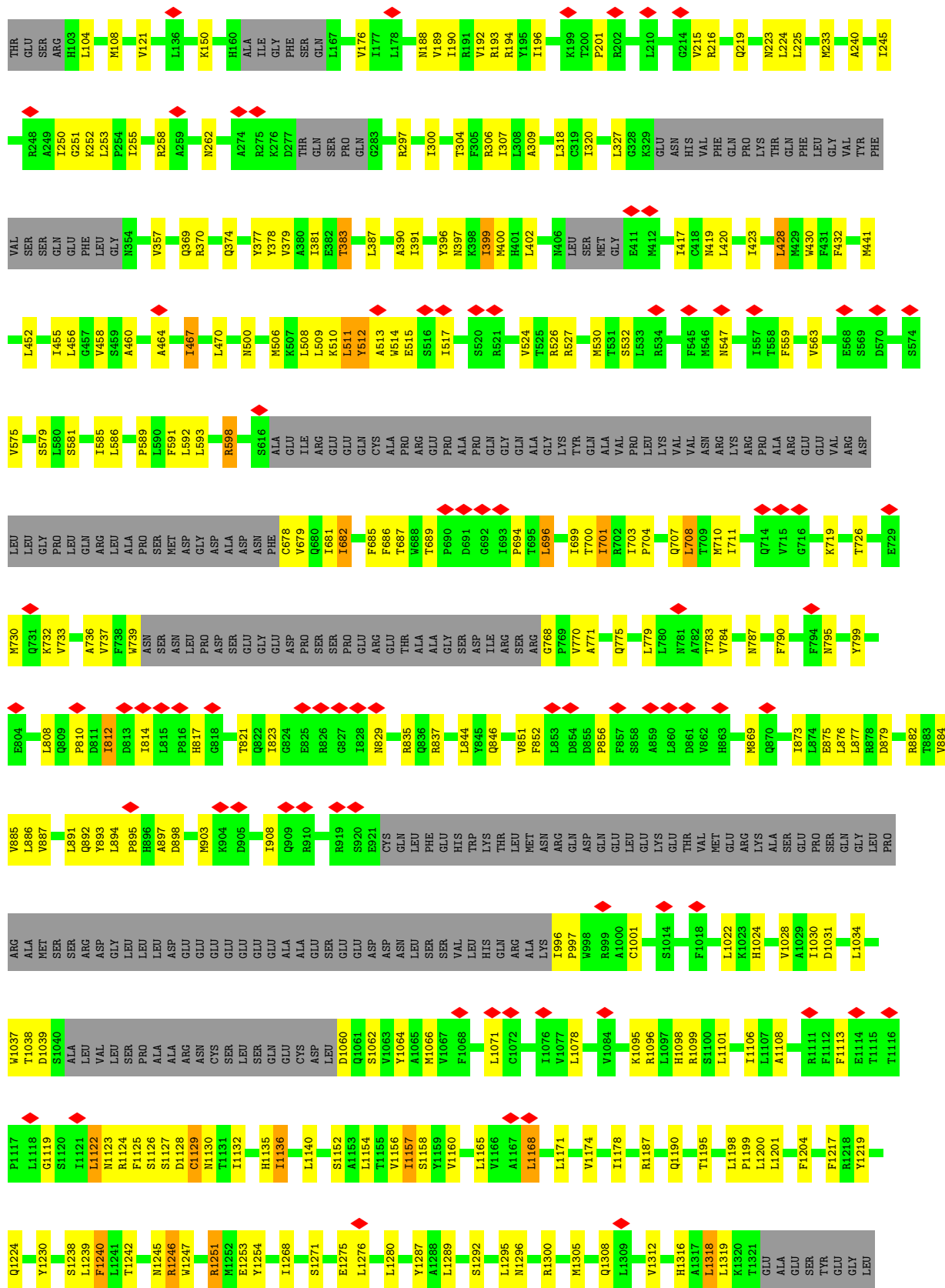
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

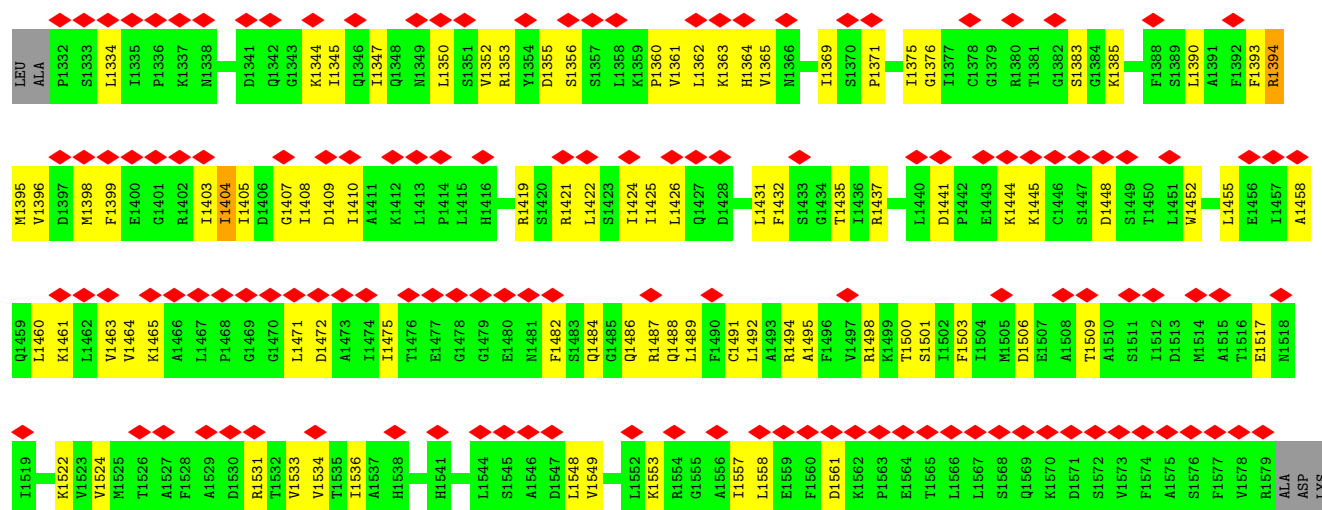


- [illegible]

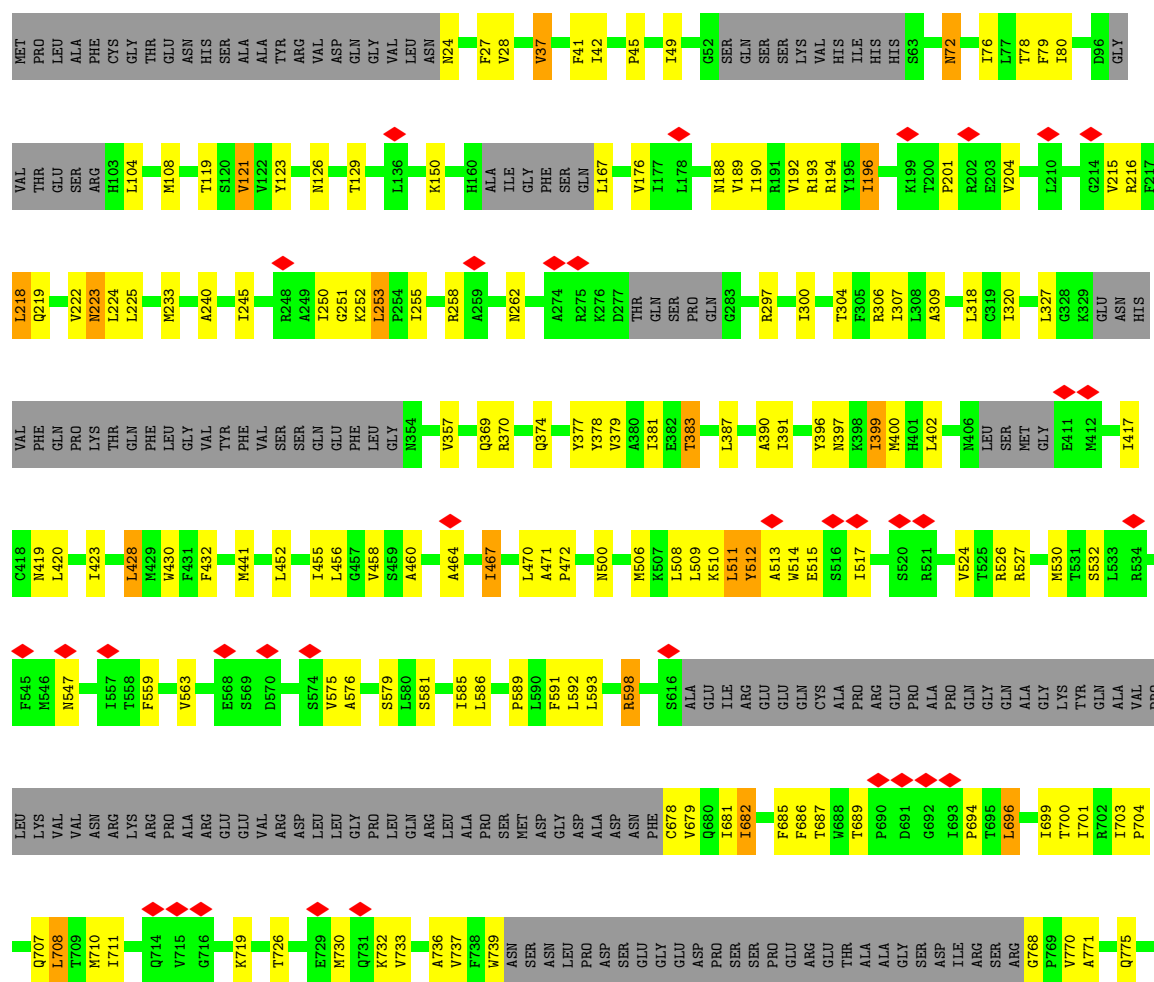
- [illegible]

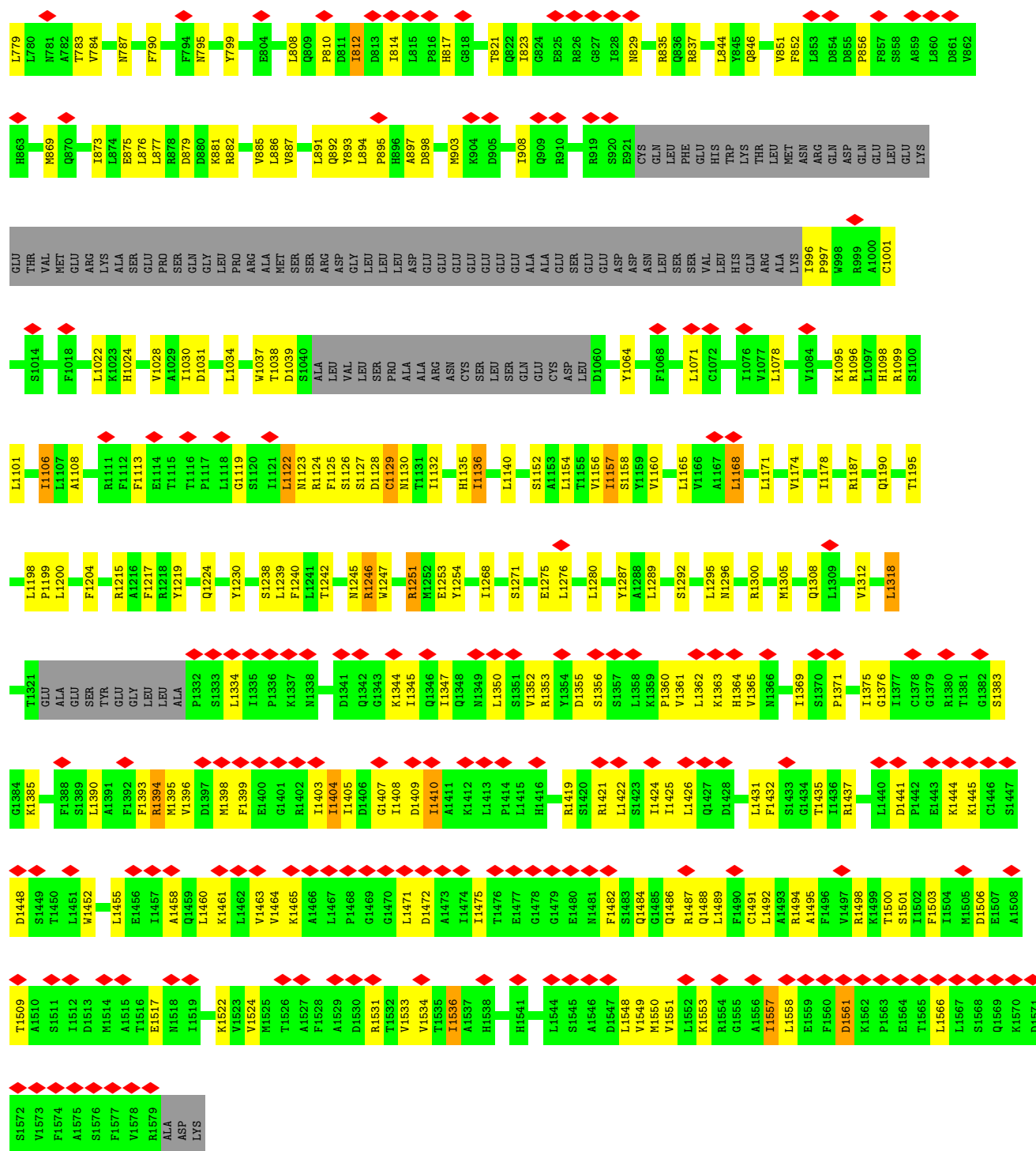
- Chain B:
-
- | Amino Acid Type | Percentage |
|-----------------|------------|
| Red | 13% |
| Green | 60% |
| Yellow | 22% |
| Grey | 17% |





• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

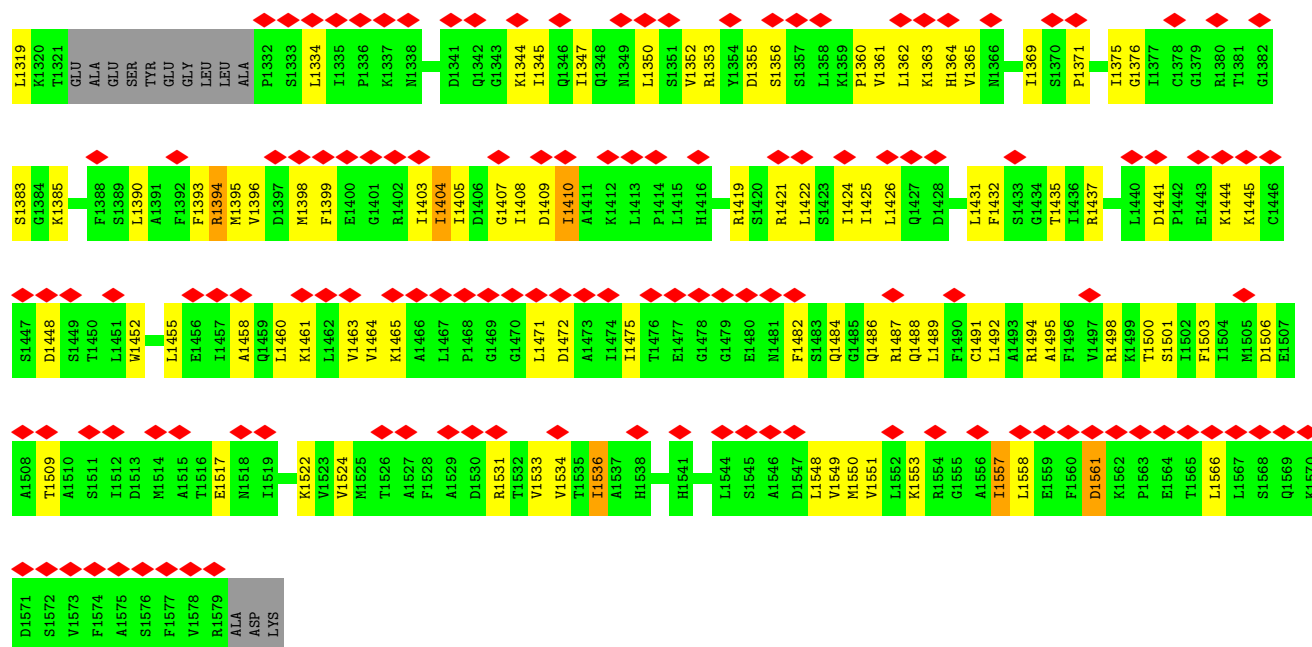




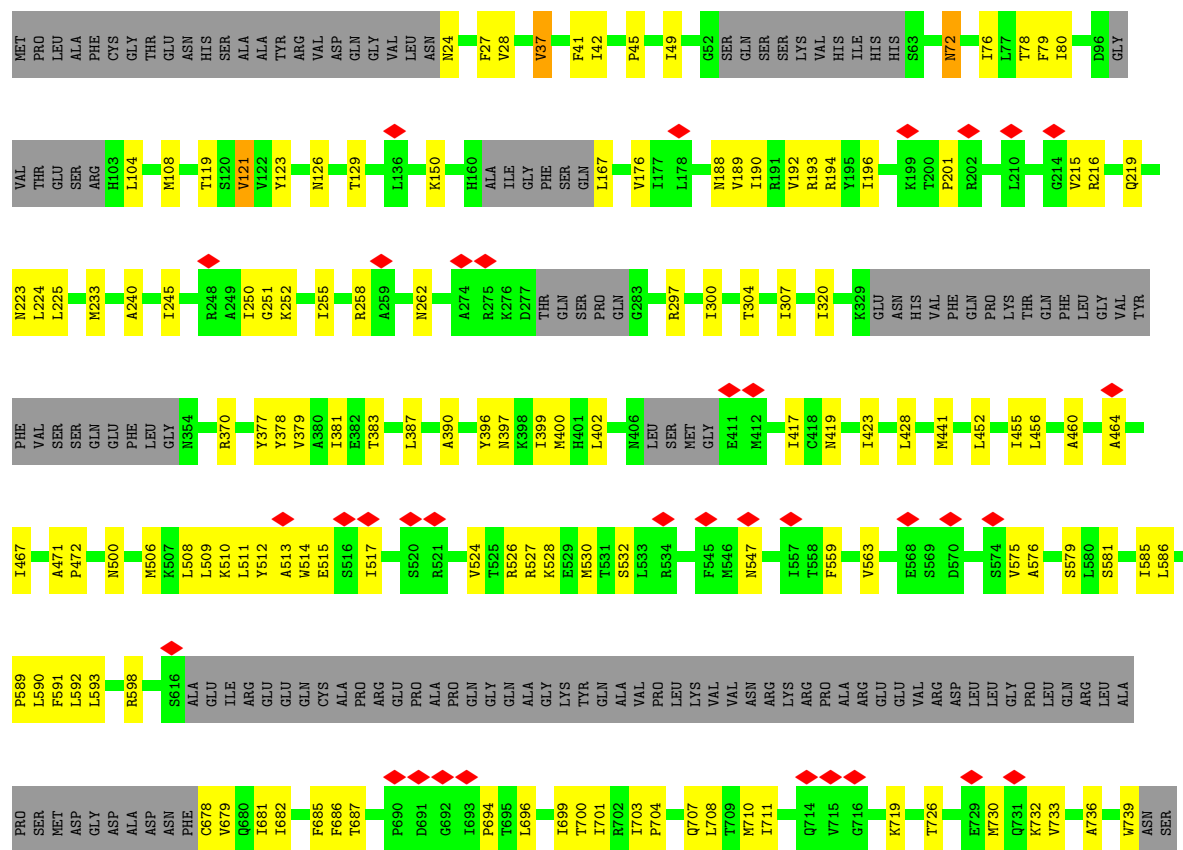
● Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2







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M1550	R1487	K1359	L1280	H1135	CYS	ASP	D898	H817	ASN
V1551	Q1488	P1360	L1289	I1136	SER	GLU	M903	Q818	LEU
K1553	L1489	L1362	L1289	L1140	SER	GLU	K904	T821	PRO
R1554	F1490	K1383	S1292	S1152	GLN	GLU	Q905	Q822	ASP
G1555	C1491	H1364	L1295	A1153	GLU	GLU	D905	I823	SER
A1556	L1492	V1365	L1295	A1153	CYS	GLU	I908	Q824	GLY
L1557	A1493	N1366	R1300	T1155	ASP	GLU	Q909	E825	GLU
L1558	R1494	I1369	M1305	T1156	LEU	ALA	R910	E826	ASP
F1559	F1496	S1370	Q1308	I1157	ALA	ALA	Q909	R828	PRO
F1560	V1497	P1371	L1309	S1168	SER	GLU	R919	R827	PRO
D1561	R1499	I1375	V1312	Y1159	ASP	GLU	E921	I828	PRO
K1562	T1500	I1376	H1316	V1160	ASP	ASP	CYS	N829	GLU
S1501	I1502	G1376	A1317	V1166	ASN	ASP	GLN	R835	ARG
P1563	F1503	I1377	L1318	A1167	ASN	ASP	LEU	Q836	GLU
E1564	P1442	Q1378	L1319	L1168	LEU	LEU	PHE	R837	THR
T1565	E1443	G1379	L1320	L1171	SER	SER	ALA	L844	ALA
L1566	K1444	T1381	T1321	L1171	VAL	SER	HIS	Y845	GLY
L1567	K1445	G1382	GLU	V1174	HIS	VAL	TRP	Q846	SER
S1568	G1446	S1383	ALA	V1174	GLN	GLN	LYS	V851	ARG
Q1569	S1447	G1384	GLU	R1187	ARG	ALA	THR	F852	SER
K1570	D1448	K1385	SER	Q1190	ALA	LYS	MET	L853	SER
D1571	S1511	F1388	TVR	L1198	LYS	LYS	ASN	D854	ARG
S1572	D1512	S1389	GLU	P1199	SER	P997	ARG	F855	ARG
V1573	D1513	L1390	GLU	L1200	GLN	P997	GLN	P856	LYS
F1574	M1514	A1391	LEU	L1200	ASP	Q998	ASP	F857	GLY
A1575	T1516	F1392	ALA	R1215	GLU	Q999	GLU	Q775	GLY
S1576	E1517	R1393	P1332	A1216	LEU	S1014	LEU	L779	LYS
F1577	I1518	R1394	S1333	R1216	LYS	F1018	LYS	L780	LYS
I1519	I1519	M1395	L1334	R1217	GLU	L1022	THR	N781	ASP
K1522	K1522	V1396	L1334	Y1219	LEU	K1023	VAL	A782	ASP
V1523	L1455	L1460	I1335	Q1224	GLU	H1024	GLU	T783	VAL
V1524	E1456	L1461	I1336	Q1224	GLU	Y1028	GLU	V784	VAL
M1525	I1457	A1458	P1337	Y1230	ARG	I1030	LYS	N787	ARG
T1526	A1458	Q1459	K1337	L1239	LYS	I1030	ALA	F790	LYS
A1527	L1462	E1400	R1338	F1240	SER	L1034	GLU	F794	LYS
F1528	V1464	G1401	N1338	L1241	PRO	W1037	PRO	N795	LYS
A1529	K1465	I1403	D1341	T1242	GLN	T1038	GLN	R798	GLY
D1530	A1466	I1404	Q1342	T1242	GLN	D1039	GLY	Y799	GLY
R1531	L1467	I1405	G1343	N1245	LEU	S1040	LEU	E804	LYS
T1532	P1468	D1406	K1344	R1246	PRO	ALA	PRO	L808	ARG
V1533	G1469	G1407	I1345	W1247	ALA	LEU	ARG	Q809	LEU
V1534	G1470	I1408	L1346	R1251	VAL	VAL	ALA	V885	LEU
I1536	L1471	D1409	I1347	M1252	LEU	LEU	MET	P810	LEU
A1537	D1472	I1410	Q1348	E1253	SER	SER	SER	D811	LEU
H1538	A1473	A1411	N1349	S1271	PRO	ALA	ASP	I812	LEU
H1541	L1474	K1412	L1350	E1276	ALA	ALA	GLY	D813	LEU
L1544	I1475	L1413	S1351	L1276	ARG	ASN	LEU	L815	LEU
S1545	T1476	P1414	R1353	Y1354	LEU	LEU	LEU	P816	LEU
A1546	E1477	L1415	Y1355	D1355	LEU	LEU	LEU	H896	LEU
D1547	G1478	H1416	S1356	S1357	LEU	LEU	LEU	A897	LEU
L1548	G1479	R1419	S1357	L1358	LEU	LEU	LEU		
V1549	F1482	R1421	L1422		LEU	LEU	LEU		
	S1483				LEU	LEU	LEU		
	Q1484				LEU	LEU	LEU		
	G1485				LEU	LEU	LEU		
	Q1486				LEU	LEU	LEU		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40340	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size ($\text{\AA}$)	329.15997, 329.15997, 329.15997	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.055, 1.055, 1.055	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, GBM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/2486	0.38	0/3391
1	C	0.15	0/2486	0.38	0/3391
1	E	0.15	0/2486	0.38	0/3391
1	G	0.15	0/2486	0.38	0/3391
2	B	0.18	0/10394	0.40	5/14113 (0.0%)
2	D	0.18	0/10394	0.40	5/14113 (0.0%)
2	F	0.18	0/10394	0.40	5/14113 (0.0%)
2	H	0.18	0/10394	0.40	5/14113 (0.0%)
All	All	0.18	0/51520	0.40	20/70016 (0.0%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	532	SER	CA-C-N	7.34	130.84	120.28
2	B	532	SER	C-N-CA	7.34	130.84	120.28
2	D	532	SER	CA-C-N	7.34	130.84	120.28
2	D	532	SER	C-N-CA	7.34	130.84	120.28
2	F	532	SER	CA-C-N	7.34	130.84	120.28
2	F	532	SER	C-N-CA	7.34	130.84	120.28
2	H	532	SER	CA-C-N	7.34	130.84	120.28
2	H	532	SER	C-N-CA	7.34	130.84	120.28
2	B	1404	ILE	N-CA-C	6.92	120.37	108.95
2	D	1404	ILE	N-CA-C	6.92	120.37	108.95
2	F	1404	ILE	N-CA-C	6.92	120.37	108.95
2	H	1404	ILE	N-CA-C	6.92	120.37	108.95
2	B	1448	ASP	N-CA-C	6.83	119.30	111.11
2	D	1448	ASP	N-CA-C	6.83	119.30	111.11
2	F	1448	ASP	N-CA-C	6.83	119.30	111.11
2	H	1448	ASP	N-CA-C	6.83	119.30	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1135	HIS	N-CA-C	5.71	121.67	114.31
2	D	1135	HIS	N-CA-C	5.71	121.67	114.31
2	F	1135	HIS	N-CA-C	5.71	121.67	114.31
2	H	1135	HIS	N-CA-C	5.71	121.67	114.31

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2433	0	2404	65	0
1	C	2433	0	2404	62	0
1	E	2433	0	2404	61	0
1	G	2433	0	2404	65	0
2	B	10189	0	10510	283	0
2	D	10189	0	10510	281	0
2	F	10189	0	10510	288	0
2	H	10189	0	10510	286	0
3	A	31	0	12	2	0
3	B	31	0	12	2	0
3	C	31	0	12	2	0
3	D	31	0	12	2	0
3	E	31	0	12	2	0
3	F	31	0	12	2	0
3	G	31	0	12	2	0
3	H	31	0	12	2	0
4	B	33	0	28	4	0
4	D	33	0	28	4	0
4	F	33	0	28	3	0
4	H	33	0	28	3	0
All	All	50868	0	51864	1374	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1374) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1350:LEU:HD11	2:F:1403:ILE:HD11	1.20	1.19
2:D:1350:LEU:HD11	2:D:1403:ILE:HD11	1.20	1.17
2:H:1350:LEU:HD11	2:H:1403:ILE:HD11	1.20	1.15
2:B:1350:LEU:HD11	2:B:1403:ILE:HD11	1.20	1.13
2:D:512:TYR:CB	2:D:1498:ARG:HH12	1.65	1.10
2:B:512:TYR:CB	2:B:1498:ARG:HH12	1.65	1.09
2:H:1350:LEU:HD13	2:H:1403:ILE:HG12	1.35	1.09
2:F:512:TYR:CB	2:F:1498:ARG:HH12	1.65	1.09
2:D:512:TYR:HB3	2:D:1498:ARG:NH1	1.67	1.09
2:H:512:TYR:HB3	2:H:1498:ARG:NH1	1.67	1.09
2:D:1350:LEU:HD13	2:D:1403:ILE:HG12	1.35	1.08
2:F:1350:LEU:HD13	2:F:1403:ILE:HG12	1.35	1.08
2:H:512:TYR:CB	2:H:1498:ARG:HH12	1.65	1.08
2:B:512:TYR:HB3	2:B:1498:ARG:NH1	1.67	1.08
2:D:1125:PHE:HA	2:D:1129:CYS:SG	1.95	1.07
2:F:1125:PHE:HA	2:F:1129:CYS:SG	1.95	1.06
2:B:1350:LEU:HD13	2:B:1403:ILE:HG12	1.35	1.06
2:F:512:TYR:HB3	2:F:1498:ARG:NH1	1.67	1.06
2:D:530:MET:HE3	2:D:1095:LYS:HG2	1.38	1.06
2:B:1125:PHE:HA	2:B:1129:CYS:SG	1.95	1.06
2:B:1350:LEU:HD13	2:B:1403:ILE:CG1	1.85	1.06
2:H:1125:PHE:HA	2:H:1129:CYS:SG	1.95	1.06
2:H:1350:LEU:HD13	2:H:1403:ILE:CG1	1.85	1.05
2:D:1350:LEU:HD13	2:D:1403:ILE:CG1	1.85	1.05
2:F:1350:LEU:HD13	2:F:1403:ILE:CG1	1.85	1.04
2:B:530:MET:HE3	2:B:1095:LYS:HG2	1.38	1.04
2:F:530:MET:HE3	2:F:1095:LYS:HG2	1.38	1.04
2:H:1124:ARG:HD2	2:H:1318:LEU:HD12	1.41	1.03
2:H:530:MET:HE3	2:H:1095:LYS:HG2	1.38	1.02
2:B:1494:ARG:O	2:B:1498:ARG:HG3	1.59	1.02
2:F:1494:ARG:O	2:F:1498:ARG:HG3	1.59	1.01
2:F:1124:ARG:HD2	2:F:1318:LEU:HD12	1.41	1.01
2:B:1124:ARG:HD2	2:B:1318:LEU:HD12	1.41	1.01
2:D:1494:ARG:O	2:D:1498:ARG:HG3	1.59	1.01
2:H:1494:ARG:O	2:H:1498:ARG:HG3	1.59	1.00
2:D:1124:ARG:HD2	2:D:1318:LEU:HD12	1.41	0.99
2:D:1350:LEU:CD1	2:D:1403:ILE:HD11	1.92	0.99
2:D:194:ARG:CB	2:D:201:PRO:HB3	1.92	0.99
2:B:1350:LEU:CD1	2:B:1403:ILE:HD11	1.92	0.99
2:F:1350:LEU:CD1	2:F:1403:ILE:HD11	1.92	0.98
2:B:194:ARG:CB	2:B:201:PRO:HB3	1.92	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1350:LEU:CD1	2:H:1403:ILE:HD11	1.92	0.98
2:H:194:ARG:CB	2:H:201:PRO:HB3	1.92	0.97
2:F:194:ARG:CB	2:F:201:PRO:HB3	1.92	0.97
2:B:512:TYR:CB	2:B:1498:ARG:NH1	2.27	0.96
2:D:512:TYR:CB	2:D:1498:ARG:NH1	2.27	0.94
2:H:512:TYR:CB	2:H:1498:ARG:NH1	2.27	0.94
2:B:500:ASN:OD1	2:B:1122:LEU:HD21	1.70	0.92
2:F:512:TYR:CB	2:F:1498:ARG:NH1	2.27	0.92
2:B:1350:LEU:HD11	2:B:1403:ILE:CD1	2.00	0.92
2:D:500:ASN:OD1	2:D:1122:LEU:HD21	1.70	0.92
2:D:1350:LEU:HD11	2:D:1403:ILE:CD1	2.00	0.92
2:F:530:MET:HE3	2:F:1095:LYS:CG	2.00	0.92
2:H:530:MET:HE3	2:H:1095:LYS:CG	2.00	0.92
2:H:500:ASN:OD1	2:H:1122:LEU:HD21	1.70	0.91
2:F:500:ASN:OD1	2:F:1122:LEU:HD21	1.70	0.91
2:D:530:MET:HE3	2:D:1095:LYS:CG	2.00	0.91
2:B:530:MET:HE3	2:B:1095:LYS:CG	2.00	0.90
2:F:1350:LEU:HD11	2:F:1403:ILE:CD1	2.00	0.90
2:D:512:TYR:HB3	2:D:1498:ARG:CZ	2.03	0.89
2:H:188:ASN:O	2:H:192:VAL:HG23	1.73	0.89
2:B:188:ASN:O	2:B:192:VAL:HG23	1.73	0.89
2:H:1350:LEU:HD11	2:H:1403:ILE:CD1	2.00	0.89
2:D:188:ASN:O	2:D:192:VAL:HG23	1.73	0.88
2:F:188:ASN:O	2:F:192:VAL:HG23	1.73	0.88
2:F:512:TYR:HB3	2:F:1498:ARG:CZ	2.03	0.88
2:B:512:TYR:HB3	2:B:1498:ARG:CZ	2.03	0.88
2:H:512:TYR:HB3	2:H:1498:ARG:CZ	2.03	0.88
2:H:1350:LEU:CD1	2:H:1403:ILE:CG1	2.52	0.87
2:F:1350:LEU:CD1	2:F:1403:ILE:CG1	2.52	0.87
2:B:512:TYR:CB	2:B:1498:ARG:HH22	1.87	0.87
2:F:512:TYR:CB	2:F:1498:ARG:HH22	1.87	0.87
2:D:512:TYR:CB	2:D:1498:ARG:HH22	1.87	0.86
2:B:1350:LEU:CD1	2:B:1403:ILE:CG1	2.52	0.86
2:H:512:TYR:CB	2:H:1498:ARG:HH22	1.87	0.86
2:D:1350:LEU:CD1	2:D:1403:ILE:CG1	2.52	0.85
2:F:72:ASN:HB3	2:F:224:LEU:CD1	2.09	0.83
2:B:72:ASN:HB3	2:B:224:LEU:CD1	2.09	0.83
2:D:72:ASN:HB3	2:D:224:LEU:CD1	2.09	0.83
2:D:1350:LEU:CD1	2:D:1403:ILE:CD1	2.57	0.83
2:B:79:PHE:HZ	2:B:225:LEU:HD12	1.44	0.82
2:H:72:ASN:HB3	2:H:224:LEU:CD1	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1350:LEU:CD1	2:B:1403:ILE:CD1	2.57	0.82
2:D:79:PHE:HZ	2:D:225:LEU:HD12	1.44	0.82
2:B:512:TYR:HB2	2:B:1498:ARG:HH12	1.42	0.82
2:F:72:ASN:HA	2:F:224:LEU:HD13	1.62	0.82
2:F:79:PHE:HZ	2:F:225:LEU:HD12	1.44	0.82
2:D:512:TYR:HB2	2:D:1498:ARG:HH12	1.42	0.81
2:F:512:TYR:HB2	2:F:1498:ARG:HH12	1.42	0.81
2:H:512:TYR:HB2	2:H:1498:ARG:HH12	1.42	0.81
2:D:512:TYR:CB	2:D:1498:ARG:NH2	2.44	0.81
2:F:512:TYR:CD2	2:F:1498:ARG:NH2	2.49	0.81
2:F:1350:LEU:CD1	2:F:1403:ILE:CD1	2.57	0.81
2:B:512:TYR:CB	2:B:1498:ARG:NH2	2.44	0.81
2:D:72:ASN:HA	2:D:224:LEU:HD13	1.62	0.81
2:F:512:TYR:CB	2:F:1498:ARG:NH2	2.44	0.81
2:H:72:ASN:HA	2:H:224:LEU:HD13	1.62	0.81
2:B:72:ASN:HA	2:B:224:LEU:HD13	1.62	0.81
2:B:512:TYR:CD2	2:B:1498:ARG:NH2	2.49	0.81
2:D:512:TYR:CD2	2:D:1498:ARG:NH2	2.49	0.81
2:F:1101:LEU:HD23	2:F:1125:PHE:CE1	2.16	0.81
2:H:1101:LEU:HD23	2:H:1125:PHE:CE1	2.16	0.81
2:H:512:TYR:CB	2:H:1498:ARG:NH2	2.44	0.81
2:H:512:TYR:CD2	2:H:1498:ARG:NH2	2.49	0.80
2:D:1101:LEU:HD23	2:D:1125:PHE:CE1	2.16	0.80
2:B:1101:LEU:HD23	2:B:1125:PHE:CE1	2.16	0.80
2:H:79:PHE:HZ	2:H:225:LEU:HD12	1.44	0.80
2:H:1350:LEU:CD1	2:H:1403:ILE:CD1	2.57	0.80
1:A:214:THR:HA	1:A:248:GLY:HA2	1.65	0.79
2:B:1037:TRP:CD1	2:B:1064:TYR:HB3	2.18	0.78
2:F:1037:TRP:CD1	2:F:1064:TYR:HB3	2.18	0.78
2:H:1037:TRP:CD1	2:H:1064:TYR:HB3	2.18	0.78
1:C:214:THR:HA	1:C:248:GLY:HA2	1.65	0.77
2:D:1037:TRP:CD1	2:D:1064:TYR:HB3	2.18	0.77
2:B:1132:ILE:HD11	2:B:1312:VAL:HG22	1.67	0.77
2:B:1124:ARG:CD	2:B:1318:LEU:HD12	2.15	0.77
2:D:1124:ARG:CD	2:D:1318:LEU:HD12	2.15	0.77
2:F:1124:ARG:CD	2:F:1318:LEU:HD12	2.15	0.77
2:D:1132:ILE:HD11	2:D:1312:VAL:HG22	1.67	0.77
2:B:1422:LEU:C	2:B:1500:THR:HG21	2.10	0.76
2:F:1422:LEU:C	2:F:1500:THR:HG21	2.10	0.76
2:H:1124:ARG:CD	2:H:1318:LEU:HD12	2.15	0.76
2:H:1422:LEU:C	2:H:1500:THR:HG21	2.10	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:THR:HA	1:E:248:GLY:HA2	1.65	0.76
1:G:214:THR:HA	1:G:248:GLY:HA2	1.65	0.76
2:D:1422:LEU:C	2:D:1500:THR:HG21	2.10	0.75
2:F:1132:ILE:HD11	2:F:1312:VAL:HG22	1.67	0.75
2:H:1132:ILE:HD11	2:H:1312:VAL:HG22	1.67	0.75
2:D:1125:PHE:CA	2:D:1129:CYS:SG	2.76	0.74
2:H:456:LEU:HB2	2:H:460:ALA:HB2	1.70	0.73
2:H:1125:PHE:CA	2:H:1129:CYS:SG	2.76	0.73
2:H:194:ARG:CB	2:H:201:PRO:CB	2.67	0.73
2:F:456:LEU:HB2	2:F:460:ALA:HB2	1.70	0.73
2:B:456:LEU:HB2	2:B:460:ALA:HB2	1.70	0.73
2:D:456:LEU:HB2	2:D:460:ALA:HB2	1.70	0.73
2:D:194:ARG:CB	2:D:201:PRO:CB	2.67	0.73
2:B:512:TYR:CB	2:B:1498:ARG:CZ	2.67	0.72
2:F:1125:PHE:CA	2:F:1129:CYS:SG	2.76	0.72
2:B:1441:ASP:OD2	2:B:1444:LYS:HA	1.90	0.72
2:B:194:ARG:CB	2:B:201:PRO:CB	2.67	0.72
2:B:1125:PHE:CA	2:B:1129:CYS:SG	2.76	0.72
2:F:194:ARG:CB	2:F:201:PRO:CB	2.67	0.71
2:F:1441:ASP:OD2	2:F:1444:LYS:HA	1.90	0.71
2:D:1441:ASP:OD2	2:D:1444:LYS:HA	1.90	0.71
1:E:36:VAL:HG12	1:E:42:CYS:HA	1.72	0.71
1:C:36:VAL:HG12	1:C:42:CYS:HA	1.72	0.71
2:H:512:TYR:CB	2:H:1498:ARG:CZ	2.67	0.71
2:H:1441:ASP:OD2	2:H:1444:LYS:HA	1.90	0.71
1:A:36:VAL:HG12	1:A:42:CYS:HA	1.72	0.70
1:A:219:VAL:HG13	1:A:236:VAL:HG23	1.72	0.70
2:B:1124:ARG:HD2	2:B:1318:LEU:CD1	2.21	0.70
2:D:216:ARG:HD2	2:D:250:ILE:C	2.17	0.70
2:F:1124:ARG:HD2	2:F:1318:LEU:CD1	2.21	0.70
2:F:1125:PHE:O	2:F:1129:CYS:SG	2.50	0.70
1:G:219:VAL:HG13	1:G:236:VAL:HG23	1.72	0.70
2:D:512:TYR:CB	2:D:1498:ARG:CZ	2.67	0.69
2:B:216:ARG:HD2	2:B:250:ILE:C	2.17	0.69
2:D:1125:PHE:O	2:D:1129:CYS:SG	2.50	0.69
2:H:216:ARG:HD2	2:H:250:ILE:C	2.17	0.69
1:G:36:VAL:HG12	1:G:42:CYS:HA	1.72	0.69
2:F:216:ARG:HD2	2:F:250:ILE:C	2.17	0.69
2:H:1124:ARG:HD2	2:H:1318:LEU:CD1	2.21	0.69
1:C:219:VAL:HG13	1:C:236:VAL:HG23	1.72	0.69
2:H:1125:PHE:O	2:H:1129:CYS:SG	2.50	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1125:PHE:O	2:B:1129:CYS:SG	2.50	0.69
1:E:219:VAL:HG13	1:E:236:VAL:HG23	1.72	0.69
2:F:1509:THR:HG23	2:F:1517:GLU:HG2	1.75	0.68
2:D:687:THR:HB	2:D:694:PRO:HA	1.75	0.68
2:F:512:TYR:CB	2:F:1498:ARG:CZ	2.67	0.68
2:H:687:THR:HB	2:H:694:PRO:HA	1.75	0.68
2:F:1421:ARG:HG3	2:F:1422:LEU:HG	1.76	0.68
2:B:1345:ILE:HD11	2:B:1369:ILE:HD12	1.76	0.68
2:B:1421:ARG:HG3	2:B:1422:LEU:HG	1.76	0.68
2:D:1421:ARG:HG3	2:D:1422:LEU:HG	1.76	0.68
2:B:512:TYR:CG	2:B:1498:ARG:NH2	2.62	0.68
2:F:1165:LEU:HA	2:F:1168:LEU:HD23	1.76	0.68
2:D:1165:LEU:HA	2:D:1168:LEU:HD23	1.76	0.68
2:H:1421:ARG:HG3	2:H:1422:LEU:HG	1.76	0.68
2:B:530:MET:HG3	2:B:1095:LYS:HE2	1.76	0.68
2:D:512:TYR:CG	2:D:1498:ARG:NH2	2.62	0.68
2:D:1126:SER:O	2:D:1130:ASN:ND2	2.28	0.68
2:B:687:THR:HB	2:B:694:PRO:HA	1.75	0.67
2:H:1101:LEU:HG	2:H:1125:PHE:CZ	2.29	0.67
2:H:1165:LEU:HA	2:H:1168:LEU:HD23	1.76	0.67
2:H:1509:THR:HG23	2:H:1517:GLU:HG2	1.75	0.67
2:D:530:MET:HG3	2:D:1095:LYS:HE2	1.76	0.67
2:F:530:MET:HG3	2:F:1095:LYS:HE2	1.76	0.67
2:H:72:ASN:CB	2:H:224:LEU:CD1	2.73	0.67
2:H:1126:SER:O	2:H:1130:ASN:ND2	2.28	0.67
2:D:1345:ILE:HD11	2:D:1369:ILE:HD12	1.76	0.67
2:B:72:ASN:CB	2:B:224:LEU:CD1	2.73	0.67
2:H:1345:ILE:HD11	2:H:1369:ILE:HD12	1.76	0.67
2:B:1509:THR:HG23	2:B:1517:GLU:HG2	1.75	0.67
2:D:1101:LEU:HG	2:D:1125:PHE:CZ	2.29	0.67
2:H:530:MET:HG3	2:H:1095:LYS:HE2	1.76	0.67
2:H:1125:PHE:C	2:H:1129:CYS:HG	2.01	0.67
2:B:1101:LEU:HG	2:B:1125:PHE:CZ	2.29	0.67
2:B:1165:LEU:HA	2:B:1168:LEU:HD23	1.76	0.67
2:F:1126:SER:O	2:F:1130:ASN:ND2	2.28	0.67
2:F:1441:ASP:OD2	2:F:1444:LYS:CA	2.43	0.67
2:H:1441:ASP:OD2	2:H:1444:LYS:CA	2.43	0.67
2:F:72:ASN:CB	2:F:224:LEU:CD1	2.73	0.67
2:F:1101:LEU:HG	2:F:1125:PHE:CZ	2.29	0.67
2:D:1509:THR:HG23	2:D:1517:GLU:HG2	1.75	0.67
2:F:1345:ILE:HD11	2:F:1369:ILE:HD12	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:512:TYR:HB2	2:B:1498:ARG:HH22	1.60	0.66
2:B:1126:SER:O	2:B:1130:ASN:ND2	2.28	0.66
2:D:1441:ASP:OD2	2:D:1444:LYS:CA	2.43	0.66
2:F:687:THR:HB	2:F:694:PRO:HA	1.75	0.66
2:B:1441:ASP:OD2	2:B:1444:LYS:CA	2.43	0.66
2:H:512:TYR:HB2	2:H:1498:ARG:HH22	1.60	0.66
2:D:1136:ILE:HD11	2:D:1308:GLN:HB3	1.77	0.66
2:D:1122:LEU:HD12	2:D:1122:LEU:O	1.96	0.66
2:D:72:ASN:CB	2:D:224:LEU:CD1	2.73	0.66
2:B:1122:LEU:HD12	2:B:1122:LEU:O	1.96	0.66
2:B:1136:ILE:HD11	2:B:1308:GLN:HB3	1.77	0.66
2:H:1136:ILE:HD11	2:H:1308:GLN:HB3	1.77	0.65
2:F:1122:LEU:HD12	2:F:1122:LEU:O	1.96	0.65
1:A:123:PHE:HD2	1:A:136:ARG:HG3	1.61	0.65
2:D:72:ASN:CA	2:D:224:LEU:HD13	2.26	0.65
2:D:512:TYR:HB2	2:D:1498:ARG:HH22	1.60	0.65
2:F:1404:ILE:HG23	2:F:1408:ILE:N	2.11	0.65
2:F:1491:CYS:HA	2:F:1494:ARG:HD2	1.78	0.65
2:D:1404:ILE:HG23	2:D:1408:ILE:N	2.11	0.65
2:H:1122:LEU:O	2:H:1122:LEU:HD12	1.96	0.65
2:F:1136:ILE:HD11	2:F:1308:GLN:HB3	1.77	0.65
1:G:123:PHE:HD2	1:G:136:ARG:HG3	1.61	0.65
2:H:72:ASN:CA	2:H:224:LEU:HD13	2.26	0.65
2:H:1404:ILE:HG23	2:H:1408:ILE:N	2.11	0.65
2:H:1503:PHE:HB2	2:H:1533:VAL:HG22	1.79	0.65
2:B:1503:PHE:HB2	2:B:1533:VAL:HG22	1.79	0.65
1:C:123:PHE:HD2	1:C:136:ARG:HG3	1.61	0.65
2:F:72:ASN:CA	2:F:224:LEU:HD13	2.26	0.65
2:H:1352:VAL:HA	2:H:1399:PHE:HA	1.79	0.65
2:F:512:TYR:HB2	2:F:1498:ARG:HH22	1.60	0.64
2:H:1491:CYS:HA	2:H:1494:ARG:HD2	1.78	0.64
2:B:72:ASN:CA	2:B:224:LEU:HD13	2.26	0.64
2:B:1404:ILE:HG23	2:B:1408:ILE:N	2.11	0.64
2:H:846:GLN:O	2:H:882:ARG:NH1	2.31	0.64
2:D:1352:VAL:HA	2:D:1399:PHE:HA	1.79	0.64
1:E:123:PHE:HD2	1:E:136:ARG:HG3	1.61	0.64
2:B:846:GLN:O	2:B:882:ARG:NH1	2.31	0.64
2:B:1352:VAL:HA	2:B:1399:PHE:HA	1.79	0.64
2:D:1491:CYS:HA	2:D:1494:ARG:HD2	1.78	0.64
2:F:262:ASN:HB3	2:F:390:ALA:HB2	1.80	0.64
2:H:262:ASN:HB3	2:H:390:ALA:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:452:LEU:HD11	2:F:464:ALA:HB2	1.80	0.64
2:F:1352:VAL:HA	2:F:1399:PHE:HA	1.79	0.64
2:B:1125:PHE:C	2:B:1129:CYS:HG	2.06	0.64
2:H:452:LEU:HD11	2:H:464:ALA:HB2	1.80	0.64
2:B:1491:CYS:HA	2:B:1494:ARG:HD2	1.78	0.63
2:D:72:ASN:CB	2:D:224:LEU:HD13	2.29	0.63
2:F:1503:PHE:HB2	2:F:1533:VAL:HG22	1.79	0.63
2:D:1503:PHE:HB2	2:D:1533:VAL:HG22	1.79	0.63
2:H:72:ASN:HB3	2:H:224:LEU:HD11	1.80	0.63
2:F:846:GLN:O	2:F:882:ARG:NH1	2.31	0.63
1:G:109:PRO:HG2	1:G:112:THR:HA	1.81	0.63
1:A:109:PRO:HG2	1:A:112:THR:HA	1.81	0.63
2:F:72:ASN:HB3	2:F:224:LEU:HD13	1.81	0.63
2:D:846:GLN:O	2:D:882:ARG:NH1	2.31	0.63
2:F:72:ASN:CB	2:F:224:LEU:HD13	2.29	0.62
2:F:387:LEU:HD21	2:F:428:LEU:HD22	1.81	0.62
2:H:72:ASN:HB3	2:H:224:LEU:HD13	1.81	0.62
2:D:1124:ARG:HD2	2:D:1318:LEU:CD1	2.21	0.62
2:B:72:ASN:CB	2:B:224:LEU:HD13	2.29	0.62
2:B:771:ALA:HB3	2:B:851:VAL:HG12	1.82	0.62
2:B:452:LEU:HD11	2:B:464:ALA:HB2	1.80	0.62
2:D:72:ASN:HB3	2:D:224:LEU:HD13	1.81	0.62
2:D:873:ILE:HA	2:D:877:LEU:HD12	1.81	0.62
2:F:873:ILE:HA	2:F:877:LEU:HD12	1.81	0.62
1:G:66:LEU:O	1:G:170:LYS:NZ	2.28	0.62
2:H:72:ASN:CB	2:H:224:LEU:HD13	2.29	0.62
2:H:387:LEU:HD21	2:H:428:LEU:HD22	1.81	0.62
2:H:771:ALA:HB3	2:H:851:VAL:HG12	1.82	0.62
2:B:262:ASN:HB3	2:B:390:ALA:HB2	1.80	0.62
2:B:1198:LEU:HB3	2:B:1199:PRO:HD3	1.82	0.62
2:D:262:ASN:HB3	2:D:390:ALA:HB2	1.80	0.62
2:D:452:LEU:HD11	2:D:464:ALA:HB2	1.80	0.62
2:D:783:THR:O	2:D:787:ASN:ND2	2.31	0.62
2:H:873:ILE:HA	2:H:877:LEU:HD12	1.81	0.62
2:B:682:ILE:HG23	2:B:736:ALA:HB3	1.82	0.62
2:B:873:ILE:HA	2:B:877:LEU:HD12	1.81	0.62
1:C:109:PRO:HG2	1:C:112:THR:HA	1.81	0.62
2:D:1245:ASN:OD1	2:D:1300:ARG:NH2	2.33	0.62
2:D:1404:ILE:CG2	2:D:1405:ILE:N	2.63	0.62
2:F:1101:LEU:CD2	2:F:1125:PHE:CE1	2.83	0.62
2:F:1404:ILE:HG23	2:F:1408:ILE:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1198:LEU:HB3	2:D:1199:PRO:HD3	1.82	0.62
2:B:72:ASN:HB3	2:B:224:LEU:HD11	1.80	0.61
2:H:399:ILE:HD11	2:H:417:ILE:HD13	1.82	0.61
2:H:1404:ILE:HG23	2:H:1408:ILE:H	1.64	0.61
2:B:1404:ILE:CG2	2:B:1405:ILE:N	2.63	0.61
2:D:686:PHE:HB2	2:D:732:LYS:HA	1.82	0.61
1:E:109:PRO:HG2	1:E:112:THR:HA	1.81	0.61
2:F:1198:LEU:HB3	2:F:1199:PRO:HD3	1.82	0.61
2:H:1198:LEU:HB3	2:H:1199:PRO:HD3	1.82	0.61
2:B:1506:ASP:HA	2:B:1536:ILE:HG13	1.83	0.61
2:D:682:ILE:HG23	2:D:736:ALA:HB3	1.82	0.61
2:F:1347:ILE:CG2	2:F:1403:ILE:HG12	2.30	0.61
2:H:1404:ILE:CG2	2:H:1405:ILE:N	2.63	0.61
1:A:63:LEU:HD13	1:A:74:ILE:HD13	1.82	0.61
2:D:1101:LEU:CD2	2:D:1125:PHE:CE1	2.83	0.61
2:D:1347:ILE:CG2	2:D:1403:ILE:HG12	2.30	0.61
2:F:72:ASN:HB3	2:F:224:LEU:HD11	1.80	0.61
2:F:771:ALA:HB3	2:F:851:VAL:HG12	1.82	0.61
2:H:1245:ASN:OD1	2:H:1300:ARG:NH2	2.33	0.61
2:B:1157:ILE:HD11	2:B:1168:LEU:HD22	1.82	0.61
2:D:387:LEU:HD21	2:D:428:LEU:HD22	1.81	0.61
1:G:63:LEU:HD13	1:G:74:ILE:HD13	1.82	0.61
2:B:686:PHE:HB2	2:B:732:LYS:HA	1.82	0.61
2:D:771:ALA:HB3	2:D:851:VAL:HG12	1.82	0.61
2:F:399:ILE:HD11	2:F:417:ILE:HD13	1.82	0.61
2:F:1245:ASN:OD1	2:F:1300:ARG:NH2	2.33	0.61
2:F:1404:ILE:CG2	2:F:1405:ILE:N	2.63	0.61
2:H:1101:LEU:CD2	2:H:1125:PHE:CE1	2.83	0.61
2:H:1506:ASP:HA	2:H:1536:ILE:HG13	1.83	0.61
2:B:1347:ILE:CG2	2:B:1403:ILE:HG12	2.30	0.61
2:H:547:ASN:HA	2:H:591:PHE:HZ	1.66	0.61
2:B:1245:ASN:OD1	2:B:1300:ARG:NH2	2.33	0.61
2:D:72:ASN:HB3	2:D:224:LEU:HD11	1.80	0.61
2:D:547:ASN:HA	2:D:591:PHE:HZ	1.66	0.61
2:D:1347:ILE:HG23	2:D:1403:ILE:HG23	1.83	0.61
2:D:1404:ILE:HG23	2:D:1408:ILE:H	1.64	0.61
2:B:387:LEU:HD21	2:B:428:LEU:HD22	1.81	0.61
1:C:63:LEU:HD13	1:C:74:ILE:HD13	1.82	0.61
2:H:1347:ILE:CG2	2:H:1403:ILE:HG12	2.30	0.61
2:B:1404:ILE:HG23	2:B:1408:ILE:H	1.64	0.61
2:F:547:ASN:HA	2:F:591:PHE:HZ	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:686:PHE:HB2	2:F:732:LYS:HA	1.82	0.61
1:C:213:ALA:HA	1:C:288:GLU:O	2.01	0.60
1:C:237:ASP:HB3	1:E:243:GLY:HA3	1.83	0.60
1:E:213:ALA:HA	1:E:288:GLU:O	2.01	0.60
2:F:1157:ILE:HD11	2:F:1168:LEU:HD22	1.82	0.60
2:F:1347:ILE:HG23	2:F:1403:ILE:HG23	1.83	0.60
2:H:783:THR:O	2:H:787:ASN:ND2	2.31	0.60
2:H:1157:ILE:HD11	2:H:1168:LEU:HD22	1.82	0.60
2:B:1347:ILE:HG23	2:B:1403:ILE:HG23	1.83	0.60
2:D:563:VAL:HG21	2:D:1037:TRP:HH2	1.67	0.60
1:E:63:LEU:HD13	1:E:74:ILE:HD13	1.82	0.60
1:E:237:ASP:HB3	1:G:243:GLY:HA3	1.83	0.60
2:H:682:ILE:HG23	2:H:736:ALA:HB3	1.82	0.60
2:H:1347:ILE:HG23	2:H:1403:ILE:HG23	1.83	0.60
2:B:1096:ARG:HG2	2:B:1099:ARG:HH12	1.67	0.60
2:B:1101:LEU:CD2	2:B:1125:PHE:CE1	2.83	0.60
2:F:1506:ASP:HA	2:F:1536:ILE:HG13	1.83	0.60
1:G:213:ALA:HA	1:G:288:GLU:O	2.01	0.60
2:H:563:VAL:HG21	2:H:1037:TRP:HH2	1.67	0.60
1:A:312:GLY:O	1:A:313:GLN:NE2	2.35	0.60
2:B:377:TYR:O	2:B:381:ILE:HG12	2.02	0.60
2:B:547:ASN:HA	2:B:591:PHE:HZ	1.66	0.60
2:D:377:TYR:O	2:D:381:ILE:HG12	2.02	0.60
2:H:686:PHE:HB2	2:H:732:LYS:HA	1.82	0.60
2:D:1157:ILE:HD11	2:D:1168:LEU:HD22	1.82	0.60
1:E:312:GLY:O	1:E:313:GLN:NE2	2.35	0.60
2:B:563:VAL:HG21	2:B:1037:TRP:HH2	1.67	0.60
2:F:682:ILE:HG23	2:F:736:ALA:HB3	1.82	0.60
2:B:399:ILE:HD11	2:B:417:ILE:HD13	1.82	0.60
1:C:95:PHE:HD1	1:C:100:LEU:HD23	1.67	0.60
2:F:1096:ARG:HG2	2:F:1099:ARG:HH12	1.67	0.60
2:F:1125:PHE:C	2:F:1129:CYS:HG	2.10	0.60
1:G:95:PHE:HD1	1:G:100:LEU:HD23	1.67	0.60
2:D:399:ILE:HD11	2:D:417:ILE:HD13	1.82	0.60
2:F:783:THR:O	2:F:787:ASN:ND2	2.31	0.60
2:F:377:TYR:O	2:F:381:ILE:HG12	2.02	0.59
2:F:563:VAL:HG21	2:F:1037:TRP:HH2	1.67	0.59
2:B:783:THR:O	2:B:787:ASN:ND2	2.31	0.59
2:D:1125:PHE:C	2:D:1129:CYS:HG	2.10	0.59
2:F:1344:LYS:HB2	2:F:1371:PRO:HG3	1.83	0.59
2:H:1096:ARG:HG2	2:H:1099:ARG:HH12	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PHE:HD1	1:A:100:LEU:HD23	1.67	0.59
1:A:213:ALA:HA	1:A:288:GLU:O	2.01	0.59
1:C:312:GLY:O	1:C:313:GLN:NE2	2.35	0.59
2:D:1506:ASP:HA	2:D:1536:ILE:HG13	1.83	0.59
2:H:1344:LYS:HB2	2:H:1371:PRO:HG3	1.83	0.59
1:A:237:ASP:HB3	1:C:243:GLY:HA3	1.83	0.59
2:B:1125:PHE:HA	2:B:1129:CYS:HG	1.66	0.59
1:G:312:GLY:O	1:G:313:GLN:NE2	2.35	0.59
1:A:243:GLY:HA3	1:G:237:ASP:HB3	1.83	0.59
2:D:1344:LYS:HB2	2:D:1371:PRO:HG3	1.83	0.59
2:B:510:LYS:O	2:B:1419:ARG:NH1	2.35	0.59
1:E:95:PHE:HD1	1:E:100:LEU:HD23	1.67	0.59
2:B:1124:ARG:HA	2:B:1128:ASP:OD2	2.03	0.59
2:D:1352:VAL:HG13	2:D:1361:VAL:HB	1.84	0.59
2:H:194:ARG:CB	2:H:201:PRO:CA	2.81	0.59
2:H:1362:LEU:HD13	2:H:1365:VAL:HG21	1.85	0.59
2:B:1501:SER:HA	2:B:1531:ARG:HD3	1.85	0.59
2:D:510:LYS:O	2:D:1419:ARG:NH1	2.35	0.59
2:F:510:LYS:O	2:F:1419:ARG:NH1	2.35	0.59
2:H:377:TYR:O	2:H:381:ILE:HG12	2.02	0.59
2:B:399:ILE:HA	2:B:402:LEU:HD23	1.85	0.58
2:B:1345:ILE:HG12	2:B:1369:ILE:HB	1.85	0.58
2:D:1096:ARG:HG2	2:D:1099:ARG:HH12	1.67	0.58
2:F:1271:SER:HA	2:F:1275:GLU:HB3	1.85	0.58
2:F:1124:ARG:HA	2:F:1128:ASP:OD2	2.03	0.58
2:H:510:LYS:O	2:H:1419:ARG:NH1	2.35	0.58
2:H:686:PHE:HD1	2:H:733:VAL:HG23	1.69	0.58
2:B:304:THR:HA	2:B:307:ILE:HG22	1.85	0.58
2:B:1344:LYS:HB2	2:B:1371:PRO:HG3	1.83	0.58
2:F:304:THR:HA	2:F:307:ILE:HG22	1.85	0.58
2:H:1125:PHE:HA	2:H:1129:CYS:HG	1.66	0.58
2:B:686:PHE:HD1	2:B:733:VAL:HG23	1.69	0.58
2:D:1271:SER:HA	2:D:1275:GLU:HB3	1.85	0.58
2:F:1352:VAL:HG13	2:F:1361:VAL:HB	1.84	0.58
2:H:1390:LEU:HB3	2:H:1395:MET:HB2	1.86	0.58
2:H:399:ILE:HA	2:H:402:LEU:HD23	1.85	0.58
2:D:194:ARG:CB	2:D:201:PRO:CA	2.81	0.58
2:D:304:THR:HA	2:D:307:ILE:HG22	1.85	0.58
2:D:399:ILE:HA	2:D:402:LEU:HD23	1.85	0.58
2:F:194:ARG:CB	2:F:201:PRO:CA	2.81	0.58
2:B:1352:VAL:HG13	2:B:1361:VAL:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1334:LEU:HD13	2:D:1408:ILE:HG12	1.86	0.58
2:H:1124:ARG:HA	2:H:1128:ASP:OD2	2.03	0.58
2:H:1345:ILE:HG12	2:H:1369:ILE:HB	1.85	0.58
2:B:194:ARG:CB	2:B:201:PRO:CA	2.81	0.58
2:D:1124:ARG:HA	2:D:1128:ASP:OD2	2.03	0.58
2:D:1362:LEU:HD13	2:D:1365:VAL:HG21	1.85	0.58
2:H:1125:PHE:CA	2:H:1129:CYS:HG	2.16	0.58
2:F:1362:LEU:HD13	2:F:1365:VAL:HG21	1.85	0.58
2:F:1393:PHE:CZ	2:F:1422:LEU:HB2	2.39	0.58
2:D:1501:SER:HA	2:D:1531:ARG:HD3	1.85	0.57
2:F:1345:ILE:HG12	2:F:1369:ILE:HB	1.85	0.57
2:H:304:THR:HA	2:H:307:ILE:HG22	1.85	0.57
2:H:1548:LEU:HG	2:H:1561:ASP:HA	1.86	0.57
2:B:1119:GLY:O	2:B:1123:ASN:HB2	2.04	0.57
2:B:1362:LEU:HD13	2:B:1365:VAL:HG21	1.85	0.57
2:D:1393:PHE:CZ	2:D:1422:LEU:HB2	2.39	0.57
2:H:512:TYR:CG	2:H:1498:ARG:NH2	2.62	0.57
2:H:1119:GLY:O	2:H:1123:ASN:HB2	2.04	0.57
2:H:1501:SER:HA	2:H:1531:ARG:HD3	1.85	0.57
2:F:686:PHE:HD1	2:F:733:VAL:HG23	1.69	0.57
2:F:1119:GLY:O	2:F:1123:ASN:HB2	2.04	0.57
2:H:1352:VAL:HG13	2:H:1361:VAL:HB	1.84	0.57
2:B:1271:SER:HA	2:B:1275:GLU:HB3	1.85	0.57
2:B:1390:LEU:HB3	2:B:1395:MET:HB2	1.86	0.57
2:B:1393:PHE:CZ	2:B:1422:LEU:HB2	2.39	0.57
2:D:512:TYR:HB3	2:D:1498:ARG:NH2	2.16	0.57
2:D:1125:PHE:HA	2:D:1129:CYS:HG	1.66	0.57
2:F:399:ILE:HA	2:F:402:LEU:HD23	1.85	0.57
2:F:512:TYR:CG	2:F:1498:ARG:NH2	2.62	0.57
2:F:1334:LEU:HD13	2:F:1408:ILE:HG12	1.86	0.57
2:F:1548:LEU:HG	2:F:1561:ASP:HA	1.86	0.57
2:H:1334:LEU:HD13	2:H:1408:ILE:HG12	1.86	0.57
2:B:1334:LEU:HD13	2:B:1408:ILE:HG12	1.86	0.57
1:E:130:THR:HA	1:G:131:ILE:HG22	1.86	0.57
2:F:216:ARG:HB2	2:F:251:GLY:HA3	1.87	0.57
2:F:1390:LEU:HB3	2:F:1395:MET:HB2	1.86	0.57
2:F:1501:SER:HA	2:F:1531:ARG:HD3	1.85	0.57
2:H:1393:PHE:CZ	2:H:1422:LEU:HB2	2.39	0.57
2:D:686:PHE:HD1	2:D:733:VAL:HG23	1.69	0.57
2:D:1119:GLY:O	2:D:1123:ASN:HB2	2.04	0.57
2:D:1345:ILE:HG12	2:D:1369:ILE:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:844:LEU:HD21	2:F:876:LEU:HD23	1.87	0.57
2:H:512:TYR:HB3	2:H:1498:ARG:NH2	2.16	0.57
2:B:1125:PHE:CA	2:B:1129:CYS:HG	2.18	0.57
1:E:66:LEU:O	1:E:170:LYS:NZ	2.28	0.57
2:H:844:LEU:HD21	2:H:876:LEU:HD23	1.87	0.57
2:D:216:ARG:HB2	2:D:251:GLY:HA3	1.87	0.56
1:A:130:THR:HA	1:C:131:ILE:HG22	1.86	0.56
2:B:72:ASN:HB3	2:B:224:LEU:HD13	1.81	0.56
2:H:1271:SER:HA	2:H:1275:GLU:HB3	1.85	0.56
3:A:401:AGS:O2A	3:A:401:AGS:H8	2.06	0.56
1:C:130:THR:HA	1:E:131:ILE:HG22	1.86	0.56
1:A:131:ILE:HG22	1:G:130:THR:HA	1.86	0.56
2:B:1422:LEU:O	2:B:1500:THR:HG21	2.05	0.56
1:C:352:ASP:O	1:C:356:LEU:N	2.39	0.56
2:D:1390:LEU:HB3	2:D:1395:MET:HB2	1.86	0.56
1:E:64:VAL:HG11	1:E:166:CYS:HB2	1.88	0.56
1:E:352:ASP:O	1:E:356:LEU:N	2.39	0.56
2:H:1422:LEU:O	2:H:1500:THR:HG21	2.05	0.56
2:B:512:TYR:HB2	2:B:1498:ARG:NH1	2.11	0.56
2:B:1344:LYS:HA	2:B:1369:ILE:O	2.06	0.56
2:B:1548:LEU:HG	2:B:1561:ASP:HA	1.86	0.56
1:C:64:VAL:HG11	1:C:166:CYS:HB2	1.88	0.56
1:C:66:LEU:O	1:C:170:LYS:NZ	2.28	0.56
3:C:401:AGS:O2A	3:C:401:AGS:H8	2.06	0.56
1:A:352:ASP:O	1:A:356:LEU:N	2.39	0.56
2:B:1251:ARG:HH11	2:B:1251:ARG:HB2	1.71	0.56
2:D:1422:LEU:O	2:D:1500:THR:HG21	2.05	0.56
2:D:1251:ARG:HB2	2:D:1251:ARG:HH11	1.71	0.56
1:E:34:ARG:HG2	1:E:305:LEU:HD21	1.88	0.56
2:F:1344:LYS:HA	2:F:1369:ILE:O	2.06	0.56
1:G:352:ASP:O	1:G:356:LEU:N	2.39	0.56
2:H:559:PHE:HE2	2:H:1034:LEU:HD11	1.71	0.56
1:A:66:LEU:O	1:A:170:LYS:NZ	2.28	0.56
2:D:1548:LEU:HG	2:D:1561:ASP:HA	1.86	0.56
2:B:844:LEU:HD21	2:B:876:LEU:HD23	1.87	0.55
2:D:844:LEU:HD21	2:D:876:LEU:HD23	1.87	0.55
3:E:401:AGS:O2A	3:E:401:AGS:H8	2.06	0.55
2:F:1158:SER:HB2	2:F:1165:LEU:HD12	1.88	0.55
2:F:1125:PHE:HA	2:F:1129:CYS:HG	1.66	0.55
2:F:1422:LEU:O	2:F:1500:THR:HG21	2.05	0.55
1:G:64:VAL:HG11	1:G:166:CYS:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:401:AGS:H8	3:G:401:AGS:O2A	2.06	0.55
2:H:1251:ARG:HH11	2:H:1251:ARG:HB2	1.71	0.55
2:H:1495:ALA:HB1	2:H:1503:PHE:HE2	1.72	0.55
2:B:216:ARG:HB2	2:B:251:GLY:HA3	1.87	0.55
2:F:512:TYR:HB3	2:F:1498:ARG:NH2	2.16	0.55
2:F:1251:ARG:HB2	2:F:1251:ARG:HH11	1.71	0.55
2:H:699:ILE:HG23	2:H:908:ILE:HD11	1.89	0.55
2:B:467:ILE:HD12	2:B:586:LEU:HD22	1.88	0.55
2:B:1127:SER:O	2:B:1128:ASP:C	2.50	0.55
2:B:1495:ALA:HB1	2:B:1503:PHE:HE2	1.72	0.55
2:D:196:ILE:O	2:D:196:ILE:HG22	2.07	0.55
2:D:467:ILE:HD12	2:D:586:LEU:HD22	1.88	0.55
2:F:1125:PHE:CA	2:F:1129:CYS:HG	2.19	0.55
2:H:1127:SER:O	2:H:1128:ASP:C	2.50	0.55
2:D:514:TRP:CZ2	2:D:1498:ARG:NH2	2.75	0.55
2:D:681:ILE:O	2:D:700:THR:HA	2.07	0.55
2:D:1495:ALA:HB1	2:D:1503:PHE:HE2	1.72	0.55
2:F:514:TRP:CZ2	2:F:1498:ARG:NH2	2.75	0.55
2:B:559:PHE:HE2	2:B:1034:LEU:HD11	1.71	0.55
2:D:1344:LYS:HA	2:D:1369:ILE:O	2.06	0.55
2:F:196:ILE:O	2:F:196:ILE:HG22	2.07	0.55
2:H:1344:LYS:HA	2:H:1369:ILE:O	2.06	0.55
1:A:34:ARG:HG2	1:A:305:LEU:HD21	1.88	0.55
2:D:1158:SER:HB2	2:D:1165:LEU:HD12	1.88	0.55
2:F:699:ILE:HG23	2:F:908:ILE:HD11	1.89	0.55
1:G:34:ARG:HG2	1:G:305:LEU:HD21	1.88	0.55
2:H:1347:ILE:HG21	2:H:1350:LEU:HD22	1.89	0.55
1:A:64:VAL:HG11	1:A:166:CYS:HB2	1.88	0.55
2:B:681:ILE:O	2:B:700:THR:HA	2.07	0.55
2:B:699:ILE:HG23	2:B:908:ILE:HD11	1.89	0.55
2:F:1435:THR:HB	2:F:1472:ASP:HA	1.89	0.55
2:F:1495:ALA:HB1	2:F:1503:PHE:HE2	1.72	0.55
2:H:514:TRP:CZ2	2:H:1498:ARG:NH2	2.75	0.55
1:C:34:ARG:HG2	1:C:305:LEU:HD21	1.88	0.54
2:H:216:ARG:HB2	2:H:251:GLY:HA3	1.87	0.54
2:F:1347:ILE:HG21	2:F:1350:LEU:HD22	1.89	0.54
2:B:514:TRP:CZ2	2:B:1498:ARG:NH2	2.75	0.54
2:D:1353:ARG:HG2	2:D:1360:PRO:HA	1.89	0.54
2:B:196:ILE:HG22	2:B:196:ILE:O	2.07	0.54
2:F:1461:LYS:HE2	2:F:1465:LYS:HE2	1.89	0.54
2:H:1158:SER:HB2	2:H:1165:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1292:SER:HA	2:H:1295:LEU:HD12	1.90	0.54
2:B:707:GLN:HG3	2:B:898:ASP:HB2	1.90	0.54
2:B:1292:SER:HA	2:B:1295:LEU:HD12	1.90	0.54
1:A:83:TRP:CD1	1:A:128:GLN:HG2	2.43	0.54
2:B:397:ASN:OD1	2:B:1224:GLN:NE2	2.41	0.54
2:B:1347:ILE:HG21	2:B:1350:LEU:HD22	1.89	0.54
2:D:686:PHE:CD2	2:D:730:MET:HB3	2.43	0.54
2:F:467:ILE:HD12	2:F:586:LEU:HD22	1.88	0.54
2:F:559:PHE:HE2	2:F:1034:LEU:HD11	1.71	0.54
2:F:1350:LEU:HB3	2:F:1365:VAL:HB	1.90	0.54
2:H:196:ILE:HG22	2:H:196:ILE:O	2.07	0.54
2:H:512:TYR:HB2	2:H:1498:ARG:NH1	2.11	0.54
2:H:686:PHE:CD2	2:H:730:MET:HB3	2.43	0.54
2:H:1350:LEU:HB3	2:H:1365:VAL:HB	1.90	0.54
2:B:1158:SER:HB2	2:B:1165:LEU:HD12	1.88	0.54
2:D:1461:LYS:HE2	2:D:1465:LYS:HE2	1.89	0.54
2:F:686:PHE:CD2	2:F:730:MET:HB3	2.43	0.54
1:G:83:TRP:CD1	1:G:128:GLN:HG2	2.43	0.54
2:H:1435:THR:HB	2:H:1472:ASP:HA	1.89	0.54
2:D:1127:SER:O	2:D:1128:ASP:C	2.50	0.54
2:D:1347:ILE:HG23	2:D:1403:ILE:HG12	1.90	0.54
2:F:1353:ARG:HG2	2:F:1360:PRO:HA	1.89	0.54
2:B:1353:ARG:HG2	2:B:1360:PRO:HA	1.89	0.54
2:D:699:ILE:HG23	2:D:908:ILE:HD11	1.89	0.54
2:D:1125:PHE:CA	2:D:1129:CYS:HG	2.19	0.54
2:F:1127:SER:O	2:F:1128:ASP:C	2.50	0.54
2:D:79:PHE:CZ	2:D:225:LEU:HD12	2.35	0.53
2:F:589:PRO:HA	2:F:592:LEU:HD12	1.90	0.53
2:F:707:GLN:HG3	2:F:898:ASP:HB2	1.90	0.53
2:B:1435:THR:HB	2:B:1472:ASP:HA	1.89	0.53
1:C:60:PHE:O	1:C:64:VAL:HG13	2.08	0.53
2:D:397:ASN:OD1	2:D:1224:GLN:NE2	2.41	0.53
2:D:1292:SER:HA	2:D:1295:LEU:HD12	1.90	0.53
2:D:1435:THR:HB	2:D:1472:ASP:HA	1.89	0.53
2:B:1347:ILE:HG23	2:B:1403:ILE:HG12	1.90	0.53
2:B:1350:LEU:HB3	2:B:1365:VAL:HB	1.90	0.53
1:E:83:TRP:CD1	1:E:128:GLN:HG2	2.43	0.53
2:F:681:ILE:O	2:F:700:THR:HA	2.07	0.53
2:H:467:ILE:HD12	2:H:586:LEU:HD22	1.88	0.53
2:B:686:PHE:CD2	2:B:730:MET:HB3	2.43	0.53
1:C:83:TRP:CD1	1:C:128:GLN:HG2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:524:VAL:HG22	2:D:527:ARG:HH12	1.74	0.53
2:F:1345:ILE:HG22	2:F:1405:ILE:HA	1.91	0.53
2:D:1345:ILE:HG22	2:D:1405:ILE:HA	1.91	0.53
2:D:1347:ILE:HG21	2:D:1350:LEU:HD22	1.89	0.53
1:G:60:PHE:O	1:G:64:VAL:HG13	2.08	0.53
2:H:397:ASN:OD1	2:H:1224:GLN:NE2	2.41	0.53
2:H:681:ILE:O	2:H:700:THR:HA	2.07	0.53
1:A:60:PHE:O	1:A:64:VAL:HG13	2.08	0.53
2:B:456:LEU:HD11	2:B:579:SER:HB3	1.91	0.53
2:B:524:VAL:HG22	2:B:527:ARG:HH12	1.74	0.53
2:B:589:PRO:HA	2:B:592:LEU:HD12	1.90	0.53
2:D:707:GLN:HG3	2:D:898:ASP:HB2	1.90	0.53
2:F:397:ASN:OD1	2:F:1224:GLN:NE2	2.41	0.53
2:F:1292:SER:HA	2:F:1295:LEU:HD12	1.90	0.53
2:B:1461:LYS:HE2	2:B:1465:LYS:HE2	1.89	0.53
2:D:1160:VAL:HG13	2:D:1280:LEU:HB3	1.91	0.53
2:H:1160:VAL:HG13	2:H:1280:LEU:HB3	1.91	0.53
2:H:1345:ILE:HG22	2:H:1405:ILE:HA	1.91	0.53
2:H:1461:LYS:HE2	2:H:1465:LYS:HE2	1.89	0.53
2:H:1463:VAL:HG21	2:H:1486:GLN:HE22	1.74	0.53
2:D:559:PHE:HE2	2:D:1034:LEU:HD11	1.71	0.53
2:D:1350:LEU:HB3	2:D:1365:VAL:HB	1.90	0.53
2:B:419:ASN:O	2:B:423:ILE:HG13	2.09	0.53
1:E:60:PHE:O	1:E:64:VAL:HG13	2.08	0.53
2:F:524:VAL:HG22	2:F:527:ARG:HH12	1.74	0.53
2:F:1125:PHE:C	2:F:1129:CYS:SG	2.92	0.53
2:F:1463:VAL:HG21	2:F:1486:GLN:HE22	1.74	0.53
2:H:1246:ARG:HH11	2:H:1246:ARG:HA	1.74	0.53
2:B:1246:ARG:HA	2:B:1246:ARG:HH11	1.74	0.53
2:B:1345:ILE:HG22	2:B:1405:ILE:HA	1.91	0.53
2:F:419:ASN:O	2:F:423:ILE:HG13	2.09	0.53
2:F:1160:VAL:HG13	2:F:1280:LEU:HB3	1.91	0.53
2:H:456:LEU:HD11	2:H:579:SER:HB3	1.91	0.53
2:D:1484:GLN:OE1	2:D:1487:ARG:NH2	2.43	0.52
2:F:1484:GLN:OE1	2:F:1487:ARG:NH2	2.43	0.52
2:D:1246:ARG:HA	2:D:1246:ARG:HH11	1.74	0.52
2:F:686:PHE:H	2:F:696:LEU:HB3	1.74	0.52
2:F:1246:ARG:HA	2:F:1246:ARG:HH11	1.74	0.52
2:H:524:VAL:HG22	2:H:527:ARG:HH12	1.74	0.52
2:H:686:PHE:H	2:H:696:LEU:HB3	1.74	0.52
2:H:1353:ARG:HG2	2:H:1360:PRO:HA	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:685:PHE:HD2	2:D:733:VAL:HB	1.75	0.52
2:D:686:PHE:H	2:D:696:LEU:HB3	1.74	0.52
2:F:456:LEU:HD11	2:F:579:SER:HB3	1.91	0.52
2:F:1347:ILE:HG23	2:F:1403:ILE:HG12	1.90	0.52
2:H:419:ASN:O	2:H:423:ILE:HG13	2.09	0.52
2:B:686:PHE:H	2:B:696:LEU:HB3	1.74	0.52
2:D:1125:PHE:C	2:D:1129:CYS:SG	2.92	0.52
2:B:1160:VAL:HG13	2:B:1280:LEU:HB3	1.91	0.52
2:H:1347:ILE:HG23	2:H:1403:ILE:HG12	1.90	0.52
2:D:808:LEU:HD13	2:D:837:ARG:HE	1.75	0.52
2:F:685:PHE:HD2	2:F:733:VAL:HB	1.75	0.52
2:H:216:ARG:HB2	2:H:251:GLY:CA	2.40	0.52
2:H:685:PHE:HD2	2:H:733:VAL:HB	1.75	0.52
2:B:1125:PHE:C	2:B:1129:CYS:SG	2.92	0.52
2:D:1463:VAL:HG21	2:D:1486:GLN:HE22	1.74	0.52
2:F:216:ARG:HB2	2:F:251:GLY:CA	2.40	0.52
2:H:589:PRO:HA	2:H:592:LEU:HD12	1.90	0.52
2:D:419:ASN:O	2:D:423:ILE:HG13	2.09	0.52
2:D:1404:ILE:HG12	2:D:1409:ASP:HB3	1.92	0.52
2:H:707:GLN:HG3	2:H:898:ASP:HB2	1.90	0.52
2:H:1125:PHE:C	2:H:1129:CYS:SG	2.92	0.52
2:B:1217:PHE:HB3	2:B:1219:TYR:HD2	1.75	0.52
2:B:1484:GLN:OE1	2:B:1487:ARG:NH2	2.43	0.52
2:D:589:PRO:HA	2:D:592:LEU:HD12	1.90	0.52
2:F:808:LEU:HD13	2:F:837:ARG:HE	1.75	0.52
2:H:808:LEU:HD13	2:H:837:ARG:HE	1.75	0.52
2:B:441:MET:HG2	2:B:593:LEU:HD12	1.92	0.51
2:B:1463:VAL:HG21	2:B:1486:GLN:HE22	1.74	0.51
2:D:216:ARG:HB2	2:D:251:GLY:CA	2.40	0.51
2:F:1441:ASP:OD2	2:F:1444:LYS:C	2.53	0.51
2:B:1404:ILE:HG12	2:B:1409:ASP:HB3	1.92	0.51
2:B:1441:ASP:OD2	2:B:1444:LYS:C	2.53	0.51
2:H:1217:PHE:HB3	2:H:1219:TYR:HD2	1.75	0.51
2:B:216:ARG:HB2	2:B:251:GLY:CA	2.40	0.51
2:D:441:MET:HG2	2:D:593:LEU:HD12	1.92	0.51
2:D:456:LEU:HD11	2:D:579:SER:HB3	1.91	0.51
2:H:1441:ASP:OD2	2:H:1444:LYS:C	2.53	0.51
2:B:1022:LEU:HB3	2:B:1078:LEU:HD21	1.93	0.51
2:D:1217:PHE:HB3	2:D:1219:TYR:HD2	1.75	0.51
2:B:685:PHE:HD2	2:B:733:VAL:HB	1.75	0.51
2:B:808:LEU:HD13	2:B:837:ARG:HE	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1404:ILE:HG12	2:F:1409:ASP:HB3	1.92	0.51
2:D:1404:ILE:HG22	2:D:1405:ILE:N	2.26	0.51
2:D:1441:ASP:OD2	2:D:1444:LYS:C	2.53	0.51
2:H:1484:GLN:OE1	2:H:1487:ARG:NH2	2.43	0.51
1:E:285:VAL:HG22	1:E:302:THR:HG22	1.93	0.51
2:H:441:MET:HG2	2:H:593:LEU:HD12	1.92	0.51
2:B:1350:LEU:CD1	2:B:1403:ILE:HG13	2.39	0.50
2:B:1455:LEU:HD13	2:B:1464:VAL:HG21	1.94	0.50
2:D:784:VAL:HG22	2:D:823:ILE:HD11	1.94	0.50
2:F:1455:LEU:HD13	2:F:1464:VAL:HG21	1.94	0.50
1:G:285:VAL:HG22	1:G:302:THR:HG22	1.93	0.50
2:F:784:VAL:HG22	2:F:823:ILE:HD11	1.94	0.50
2:F:1022:LEU:HB3	2:F:1078:LEU:HD21	1.93	0.50
1:E:202:VAL:HG23	1:E:251:LEU:HD21	1.94	0.50
2:F:370:ARG:HB3	2:F:1253:GLU:HG2	1.94	0.50
1:A:202:VAL:HG23	1:A:251:LEU:HD21	1.94	0.50
1:A:285:VAL:HG22	1:A:302:THR:HG22	1.93	0.50
1:C:202:VAL:HG23	1:C:251:LEU:HD21	1.94	0.50
2:D:370:ARG:HB3	2:D:1253:GLU:HG2	1.94	0.50
2:H:1404:ILE:HG12	2:H:1409:ASP:HB3	1.92	0.50
2:F:1217:PHE:HB3	2:F:1219:TYR:HD2	1.75	0.50
2:F:1385:LYS:HB2	2:F:1536:ILE:HG21	1.94	0.50
1:G:202:VAL:HG23	1:G:251:LEU:HD21	1.94	0.50
2:H:1022:LEU:HB3	2:H:1078:LEU:HD21	1.93	0.50
2:B:784:VAL:HG22	2:B:823:ILE:HD11	1.94	0.50
1:C:285:VAL:HG22	1:C:302:THR:HG22	1.93	0.50
2:D:513:ALA:HB2	2:D:1419:ARG:HG3	1.94	0.50
2:F:513:ALA:HB2	2:F:1419:ARG:HG3	1.94	0.50
2:F:869:MET:HA	2:F:873:ILE:HD12	1.94	0.50
2:H:784:VAL:HG22	2:H:823:ILE:HD11	1.94	0.50
2:H:1385:LYS:HB2	2:H:1536:ILE:HG21	1.94	0.50
2:H:1404:ILE:HG22	2:H:1405:ILE:N	2.26	0.50
2:B:233:MET:HB2	2:B:1247:TRP:CD1	2.47	0.50
2:F:441:MET:HG2	2:F:593:LEU:HD12	1.92	0.50
2:H:513:ALA:HB2	2:H:1419:ARG:HG3	1.94	0.50
3:H:2002:AGS:O2A	3:H:2002:AGS:S1G	2.70	0.50
2:B:223:ASN:OD1	2:B:223:ASN:N	2.41	0.50
2:H:1455:LEU:HD13	2:H:1464:VAL:HG21	1.94	0.50
1:A:198:PHE:HE1	1:A:200:LEU:HB2	1.77	0.50
2:B:508:LEU:HD12	2:B:1426:LEU:HD23	1.94	0.50
2:B:1404:ILE:HG22	2:B:1405:ILE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:512:TYR:HB2	2:D:1498:ARG:NH1	2.11	0.50
2:D:1022:LEU:HB3	2:D:1078:LEU:HD21	1.93	0.50
2:D:1455:LEU:HD13	2:D:1464:VAL:HG21	1.94	0.50
2:D:233:MET:HB2	2:D:1247:TRP:CD1	2.47	0.49
1:E:198:PHE:HE1	1:E:200:LEU:HB2	1.77	0.49
2:F:512:TYR:HB2	2:F:1498:ARG:NH2	2.24	0.49
2:F:1404:ILE:HG22	2:F:1405:ILE:N	2.26	0.49
2:B:513:ALA:HB2	2:B:1419:ARG:HG3	1.94	0.49
2:D:869:MET:HA	2:D:873:ILE:HD12	1.94	0.49
3:D:2002:AGS:O2A	3:D:2002:AGS:S1G	2.70	0.49
2:F:563:VAL:HG21	2:F:1037:TRP:CH2	2.47	0.49
2:H:370:ARG:HB3	2:H:1253:GLU:HG2	1.94	0.49
2:D:1385:LYS:HB2	2:D:1536:ILE:HG21	1.94	0.49
2:F:1024:HIS:O	2:F:1028:VAL:HG12	2.13	0.49
2:H:1132:ILE:CD1	2:H:1312:VAL:HG22	2.41	0.49
2:B:869:MET:HA	2:B:873:ILE:HD12	1.94	0.49
2:B:1385:LYS:HB2	2:B:1536:ILE:HG21	1.94	0.49
2:D:1350:LEU:CD1	2:D:1403:ILE:HG13	2.39	0.49
2:F:79:PHE:CZ	2:F:225:LEU:HD12	2.35	0.49
2:F:233:MET:HB2	2:F:1247:TRP:CD1	2.47	0.49
2:F:711:ILE:HB	2:F:887:VAL:HG13	1.95	0.49
3:F:2002:AGS:O2A	3:F:2002:AGS:S1G	2.70	0.49
2:H:508:LEU:HD12	2:H:1426:LEU:HD23	1.94	0.49
2:B:370:ARG:HB3	2:B:1253:GLU:HG2	1.94	0.49
3:B:2002:AGS:O2A	3:B:2002:AGS:S1G	2.70	0.49
1:C:139:THR:HG23	1:C:141:GLU:H	1.77	0.49
2:D:711:ILE:HB	2:D:887:VAL:HG13	1.95	0.49
2:H:1024:HIS:O	2:H:1028:VAL:HG12	2.13	0.49
1:C:36:VAL:HG23	1:C:303:SER:OG	2.13	0.49
1:C:198:PHE:HE1	1:C:200:LEU:HB2	1.77	0.49
1:G:220:VAL:HG12	1:G:235:GLN:HG2	1.95	0.49
1:A:220:VAL:HG12	1:A:235:GLN:HG2	1.95	0.49
2:B:711:ILE:HB	2:B:887:VAL:HG13	1.95	0.49
1:C:243:GLY:O	1:C:245:GLY:N	2.46	0.49
2:D:563:VAL:HG21	2:D:1037:TRP:CH2	2.47	0.49
2:D:1024:HIS:O	2:D:1028:VAL:HG12	2.13	0.49
2:F:215:VAL:HG13	2:F:252:LYS:O	2.13	0.49
2:F:511:LEU:HD13	2:F:1395:MET:HE2	1.94	0.49
2:F:1350:LEU:CD1	2:F:1403:ILE:HG13	2.39	0.49
2:H:255:ILE:HA	2:H:258:ARG:HE	1.78	0.49
2:B:1132:ILE:CD1	2:B:1312:VAL:HG22	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:VAL:HG12	1:E:235:GLN:HG2	1.95	0.49
1:G:198:PHE:HE1	1:G:200:LEU:HB2	1.77	0.49
1:A:50:ARG:HH21	3:C:401:AGS:C8	2.26	0.49
1:E:36:VAL:HG23	1:E:303:SER:OG	2.13	0.49
1:E:50:ARG:HH21	3:G:401:AGS:C8	2.26	0.49
2:F:512:TYR:HB2	2:F:1498:ARG:NH1	2.11	0.49
1:G:36:VAL:HG23	1:G:303:SER:OG	2.13	0.49
1:G:243:GLY:O	1:G:245:GLY:N	2.46	0.49
2:H:215:VAL:HG13	2:H:252:LYS:O	2.13	0.49
2:D:1171:LEU:O	2:D:1174:VAL:HB	2.13	0.49
2:F:255:ILE:HA	2:F:258:ARG:HE	1.78	0.49
2:H:233:MET:HB2	2:H:1247:TRP:CD1	2.47	0.49
2:H:1171:LEU:O	2:H:1174:VAL:HB	2.13	0.49
2:D:215:VAL:HG13	2:D:252:LYS:O	2.13	0.48
2:H:711:ILE:HB	2:H:887:VAL:HG13	1.95	0.48
3:A:401:AGS:C8	1:G:50:ARG:HH21	2.26	0.48
2:D:508:LEU:HD12	2:D:1426:LEU:HD23	1.94	0.48
1:E:139:THR:HG23	1:E:141:GLU:H	1.77	0.48
1:A:36:VAL:HG23	1:A:303:SER:OG	2.13	0.48
2:F:1132:ILE:CD1	2:F:1312:VAL:HG22	2.41	0.48
2:B:1495:ALA:HB1	2:B:1503:PHE:CE2	2.48	0.48
1:C:50:ARG:HH21	3:E:401:AGS:C8	2.26	0.48
1:C:220:VAL:HG12	1:C:235:GLN:HG2	1.95	0.48
2:H:1030:ILE:HA	2:H:1071:LEU:HD13	1.96	0.48
2:H:1495:ALA:HB1	2:H:1503:PHE:CE2	2.48	0.48
1:A:243:GLY:O	1:A:245:GLY:N	2.46	0.48
2:B:455:ILE:HG22	2:B:575:VAL:HG13	1.96	0.48
2:B:563:VAL:HG21	2:B:1037:TRP:CH2	2.47	0.48
2:D:1561:ASP:OD1	2:D:1561:ASP:N	2.47	0.48
2:F:1171:LEU:O	2:F:1174:VAL:HB	2.13	0.48
1:G:139:THR:HG23	1:G:141:GLU:H	1.77	0.48
2:H:511:LEU:HD13	2:H:1395:MET:HE2	1.94	0.48
2:B:1404:ILE:HG21	2:B:1407:GLY:CA	2.44	0.48
2:D:320:ILE:HD11	2:D:1289:LEU:HD13	1.95	0.48
1:E:243:GLY:O	1:E:245:GLY:N	2.46	0.48
2:H:869:MET:HA	2:H:873:ILE:HD12	1.94	0.48
2:B:511:LEU:HD13	2:B:1395:MET:HE2	1.94	0.48
2:F:559:PHE:CE2	2:F:1034:LEU:HD11	2.49	0.48
2:F:1030:ILE:HA	2:F:1071:LEU:HD13	1.96	0.48
2:F:1404:ILE:HG21	2:F:1407:GLY:CA	2.44	0.48
2:D:511:LEU:HD13	2:D:1395:MET:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:455:ILE:HG22	2:F:575:VAL:HG13	1.96	0.48
2:F:508:LEU:HD12	2:F:1426:LEU:HD23	1.94	0.48
2:H:563:VAL:HG21	2:H:1037:TRP:CH2	2.47	0.48
2:H:1431:LEU:HD23	2:H:1494:ARG:HH21	1.79	0.48
1:A:139:THR:HG23	1:A:141:GLU:H	1.77	0.48
2:B:1024:HIS:O	2:B:1028:VAL:HG12	2.13	0.48
2:B:1171:LEU:O	2:B:1174:VAL:HB	2.13	0.48
2:D:1495:ALA:HB1	2:D:1503:PHE:CE2	2.48	0.48
1:A:128:GLN:NE2	1:A:152:GLN:OE1	2.47	0.48
2:F:779:LEU:HD11	2:F:835:ARG:HG2	1.95	0.48
2:F:1431:LEU:HD23	2:F:1494:ARG:HH21	1.79	0.48
1:G:95:PHE:HE2	2:H:27:PHE:HB2	1.79	0.48
2:H:779:LEU:HD11	2:H:835:ARG:HG2	1.95	0.48
2:H:1404:ILE:HG21	2:H:1407:GLY:CA	2.44	0.48
1:A:132:GLY:HA3	1:C:131:ILE:O	2.15	0.47
2:B:1553:LYS:HE3	2:B:1558:LEU:HB2	1.96	0.47
2:D:779:LEU:HD11	2:D:835:ARG:HG2	1.95	0.47
2:D:1404:ILE:HG21	2:D:1407:GLY:CA	2.44	0.47
2:F:829:ASN:OD1	2:F:829:ASN:N	2.36	0.47
2:F:1495:ALA:HB1	2:F:1503:PHE:CE2	2.48	0.47
1:A:95:PHE:HE2	2:B:27:PHE:HB2	1.79	0.47
2:B:215:VAL:HG13	2:B:252:LYS:O	2.13	0.47
2:B:255:ILE:HA	2:B:258:ARG:HE	1.78	0.47
1:E:132:GLY:HA3	1:G:131:ILE:O	2.15	0.47
2:B:779:LEU:HD11	2:B:835:ARG:HG2	1.95	0.47
2:B:1030:ILE:HA	2:B:1071:LEU:HD13	1.96	0.47
2:B:1431:LEU:HD23	2:B:1494:ARG:HH21	1.79	0.47
2:F:775:GLN:OE1	3:F:2002:AGS:S1G	2.73	0.47
2:H:1553:LYS:HE3	2:H:1558:LEU:HB2	1.96	0.47
2:B:320:ILE:HD11	2:B:1289:LEU:HD13	1.95	0.47
1:C:95:PHE:HE2	2:D:27:PHE:HB2	1.79	0.47
2:D:775:GLN:OE1	3:D:2002:AGS:S1G	2.73	0.47
2:F:1553:LYS:HE3	2:F:1558:LEU:HB2	1.96	0.47
2:D:396:TYR:HE2	2:D:1224:GLN:HG3	1.80	0.47
2:D:1553:LYS:HE3	2:D:1558:LEU:HB2	1.96	0.47
1:E:95:PHE:HE2	2:F:27:PHE:HB2	1.79	0.47
2:H:559:PHE:CE2	2:H:1034:LEU:HD11	2.49	0.47
2:B:396:TYR:HE2	2:B:1224:GLN:HG3	1.80	0.47
2:B:559:PHE:CE2	2:B:1034:LEU:HD11	2.49	0.47
1:C:128:GLN:NE2	1:C:152:GLN:OE1	2.47	0.47
2:D:255:ILE:HA	2:D:258:ARG:HE	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:GLN:NE2	1:E:152:GLN:OE1	2.47	0.47
2:H:78:THR:HG21	2:H:121:VAL:HG23	1.97	0.47
2:H:1561:ASP:OD1	2:H:1561:ASP:N	2.47	0.47
2:B:194:ARG:CB	2:B:201:PRO:HA	2.45	0.47
2:D:1030:ILE:HA	2:D:1071:LEU:HD13	1.96	0.47
2:F:78:THR:HG21	2:F:121:VAL:HG23	1.97	0.47
2:F:320:ILE:HD11	2:F:1289:LEU:HD13	1.95	0.47
2:F:506:MET:SD	2:F:1113:PHE:HB3	2.55	0.47
2:F:1561:ASP:OD1	2:F:1561:ASP:N	2.47	0.47
1:G:128:GLN:NE2	1:G:152:GLN:OE1	2.47	0.47
2:H:455:ILE:HG22	2:H:575:VAL:HG13	1.96	0.47
2:H:1350:LEU:CD1	2:H:1403:ILE:HG13	2.39	0.47
2:B:775:GLN:OE1	3:B:2002:AGS:S1G	2.73	0.47
2:D:78:THR:HG21	2:D:121:VAL:HG23	1.97	0.47
2:D:506:MET:SD	2:D:1113:PHE:HB3	2.55	0.47
2:H:194:ARG:CB	2:H:201:PRO:HA	2.45	0.47
1:A:131:ILE:O	1:G:132:GLY:HA3	2.15	0.47
2:B:78:THR:HG21	2:B:121:VAL:HG23	1.97	0.47
1:C:132:GLY:HA3	1:E:131:ILE:O	2.15	0.47
2:D:559:PHE:CE2	2:D:1034:LEU:HD11	2.49	0.47
2:H:320:ILE:HD11	2:H:1289:LEU:HD13	1.95	0.47
2:H:710:MET:HE3	2:H:893:TYR:HB3	1.97	0.47
2:H:775:GLN:OE1	3:H:2002:AGS:S1G	2.73	0.47
2:H:829:ASN:OD1	2:H:829:ASN:N	2.36	0.47
2:B:1187:ARG:O	2:B:1190:GLN:HB3	2.15	0.47
2:B:1561:ASP:N	2:B:1561:ASP:OD1	2.47	0.47
1:C:45:ALA:HB2	1:E:325:ARG:HH11	1.80	0.47
2:F:396:TYR:HE2	2:F:1224:GLN:HG3	1.80	0.47
2:H:240:ALA:HB1	2:H:245:ILE:HD11	1.97	0.47
2:H:506:MET:SD	2:H:1113:PHE:HB3	2.55	0.47
2:H:846:GLN:HG3	2:H:1217:PHE:HE2	1.80	0.47
2:B:1458:ALA:O	2:B:1489:LEU:HG	2.15	0.46
2:B:506:MET:SD	2:B:1113:PHE:HB3	2.55	0.46
1:C:280:ASP:OD1	1:C:280:ASP:N	2.48	0.46
2:D:455:ILE:HG22	2:D:575:VAL:HG13	1.96	0.46
2:D:679:VAL:HB	2:D:703:ILE:HB	1.97	0.46
2:D:1431:LEU:HD23	2:D:1494:ARG:HH21	1.79	0.46
2:F:190:ILE:HD11	2:F:196:ILE:HB	1.98	0.46
2:F:679:VAL:HB	2:F:703:ILE:HB	1.97	0.46
2:H:190:ILE:HD11	2:H:196:ILE:HB	1.98	0.46
2:H:1458:ALA:O	2:H:1489:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ALA:HB2	1:C:325:ARG:HH11	1.80	0.46
2:B:79:PHE:CZ	2:B:225:LEU:HD12	2.35	0.46
2:B:240:ALA:HB1	2:B:245:ILE:HD11	1.97	0.46
2:B:846:GLN:HG3	2:B:1217:PHE:HE2	1.80	0.46
1:C:81:CYS:SG	2:D:41:PHE:HB3	2.56	0.46
2:D:240:ALA:HB1	2:D:245:ILE:HD11	1.97	0.46
2:D:846:GLN:HG3	2:D:1217:PHE:HE2	1.80	0.46
2:F:846:GLN:HG3	2:F:1217:PHE:HE2	1.80	0.46
1:A:81:CYS:SG	2:B:41:PHE:HB3	2.56	0.46
2:D:194:ARG:CB	2:D:201:PRO:HA	2.45	0.46
1:E:280:ASP:OD1	1:E:280:ASP:N	2.48	0.46
2:F:194:ARG:CB	2:F:201:PRO:HA	2.45	0.46
1:A:190:THR:HG22	1:A:191:LEU:H	1.81	0.46
2:B:1034:LEU:O	2:B:1038:THR:HG23	2.16	0.46
2:D:1458:ALA:O	2:D:1489:LEU:HG	2.15	0.46
2:F:710:MET:HE3	2:F:893:TYR:HB3	1.97	0.46
2:B:190:ILE:HD11	2:B:196:ILE:HB	1.98	0.46
2:B:710:MET:HE3	2:B:893:TYR:HB3	1.97	0.46
1:C:90:TRP:HA	1:C:93:ILE:HG22	1.98	0.46
1:C:190:THR:HG22	1:C:191:LEU:H	1.81	0.46
2:D:223:ASN:OD1	2:D:223:ASN:N	2.41	0.46
2:F:240:ALA:HB1	2:F:245:ILE:HD11	1.97	0.46
1:G:81:CYS:SG	2:H:41:PHE:HB3	2.56	0.46
2:H:1187:ARG:O	2:H:1190:GLN:HB3	2.15	0.46
2:D:190:ILE:HD11	2:D:196:ILE:HB	1.98	0.46
2:D:710:MET:HE3	2:D:893:TYR:HB3	1.97	0.46
2:H:1034:LEU:O	2:H:1038:THR:HG23	2.16	0.46
1:A:209:MET:HE3	1:A:209:MET:HB3	1.86	0.46
2:B:1404:ILE:HG23	2:B:1408:ILE:O	2.16	0.46
2:D:1376:GLY:O	2:D:1549:VAL:HA	2.16	0.46
2:F:996:ILE:HD12	2:F:997:PRO:HD2	1.98	0.46
2:F:1404:ILE:HG23	2:F:1408:ILE:O	2.16	0.46
1:G:90:TRP:HA	1:G:93:ILE:HG22	1.98	0.46
1:G:280:ASP:OD1	1:G:280:ASP:N	2.48	0.46
2:H:396:TYR:HE2	2:H:1224:GLN:HG3	1.80	0.46
2:D:1246:ARG:NH2	4:D:2001:GBM:H18	2.31	0.46
2:D:1375:ILE:HB	2:D:1534:VAL:HG22	1.98	0.46
1:E:81:CYS:SG	2:F:41:PHE:HB3	2.56	0.46
1:C:313:GLN:HB3	1:C:336:THR:CG2	2.46	0.46
2:D:869:MET:HE3	2:D:869:MET:HB3	1.87	0.46
1:E:45:ALA:HB2	1:G:325:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1034:LEU:O	2:F:1038:THR:HG23	2.16	0.46
2:F:1187:ARG:O	2:F:1190:GLN:HB3	2.15	0.46
2:F:1246:ARG:NH2	4:F:2001:GBM:H18	2.31	0.46
2:F:1458:ALA:O	2:F:1489:LEU:HG	2.15	0.46
2:H:1246:ARG:HA	2:H:1246:ARG:HD3	1.71	0.46
2:H:1375:ILE:HB	2:H:1534:VAL:HG22	1.98	0.46
2:H:1404:ILE:HG23	2:H:1408:ILE:O	2.16	0.46
2:B:1375:ILE:HB	2:B:1534:VAL:HG22	1.98	0.45
2:D:808:LEU:HG	2:D:812:ILE:HG12	1.99	0.45
2:D:996:ILE:HD12	2:D:997:PRO:HD2	1.98	0.45
2:D:1132:ILE:CD1	2:D:1312:VAL:HG22	2.41	0.45
2:D:1404:ILE:HG23	2:D:1408:ILE:O	2.16	0.45
1:E:313:GLN:HB3	1:E:336:THR:CG2	2.46	0.45
2:F:808:LEU:HG	2:F:812:ILE:HG12	1.99	0.45
1:A:280:ASP:OD1	1:A:280:ASP:N	2.48	0.45
2:B:1246:ARG:NH2	4:B:2001:GBM:H18	2.31	0.45
4:B:2001:GBM:H20	4:B:2001:GBM:H22	1.75	0.45
2:F:1375:ILE:HB	2:F:1534:VAL:HG22	1.98	0.45
2:F:1376:GLY:O	2:F:1549:VAL:HA	2.16	0.45
2:H:590:LEU:HD23	2:H:590:LEU:HA	1.83	0.45
2:H:1140:LEU:HD13	2:H:1305:MET:HE2	1.98	0.45
2:B:739:TRP:HE1	2:B:768:GLY:N	2.15	0.45
2:D:1034:LEU:O	2:D:1038:THR:HG23	2.16	0.45
2:D:1187:ARG:O	2:D:1190:GLN:HB3	2.15	0.45
1:G:313:GLN:HB3	1:G:336:THR:CG2	2.46	0.45
2:H:996:ILE:HD12	2:H:997:PRO:HD2	1.98	0.45
1:A:170:LYS:O	1:A:173:GLN:HG2	2.17	0.45
1:A:325:ARG:HH11	1:G:45:ALA:HB2	1.80	0.45
2:B:512:TYR:HB3	2:B:1498:ARG:NH2	2.16	0.45
2:D:1140:LEU:HD13	2:D:1305:MET:HE2	1.98	0.45
1:E:190:THR:HG22	1:E:191:LEU:H	1.81	0.45
2:F:678:CYS:HB3	2:F:704:PRO:HA	1.99	0.45
2:F:875:GLU:O	2:F:879:ASP:HB2	2.17	0.45
2:B:679:VAL:HB	2:B:703:ILE:HB	1.97	0.45
2:D:678:CYS:HB3	2:D:704:PRO:HA	1.99	0.45
2:D:739:TRP:HE1	2:D:768:GLY:N	2.15	0.45
1:E:170:LYS:O	1:E:173:GLN:HG2	2.17	0.45
1:E:313:GLN:HE22	1:E:338:LYS:HD2	1.82	0.45
2:H:679:VAL:HB	2:H:703:ILE:HB	1.97	0.45
1:A:313:GLN:HB3	1:A:336:THR:CG2	2.46	0.45
1:A:313:GLN:HE22	1:A:338:LYS:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:370:ARG:HG3	2:B:1253:GLU:CD	2.42	0.45
2:B:808:LEU:HG	2:B:812:ILE:HG12	1.99	0.45
2:B:996:ILE:HD12	2:B:997:PRO:HD2	1.98	0.45
2:D:875:GLU:O	2:D:879:ASP:HB2	2.17	0.45
1:E:90:TRP:HA	1:E:93:ILE:HG22	1.98	0.45
2:B:1039:ASP:OD1	2:B:1039:ASP:N	2.50	0.45
2:B:1140:LEU:HD13	2:B:1305:MET:HE2	1.98	0.45
2:B:1376:GLY:O	2:B:1549:VAL:HA	2.16	0.45
2:D:379:VAL:O	2:D:383:THR:OG1	2.35	0.45
2:F:1140:LEU:HD13	2:F:1305:MET:HE2	1.98	0.45
1:G:190:THR:HG22	1:G:191:LEU:H	1.81	0.45
2:H:1376:GLY:O	2:H:1549:VAL:HA	2.16	0.45
1:A:90:TRP:HA	1:A:93:ILE:HG22	1.98	0.45
2:B:678:CYS:HB3	2:B:704:PRO:HA	1.99	0.45
2:F:1369:ILE:HD13	2:F:1375:ILE:HG13	1.99	0.45
2:H:379:VAL:O	2:H:383:THR:OG1	2.35	0.45
2:H:739:TRP:HE1	2:H:768:GLY:N	2.15	0.45
2:H:1246:ARG:NH2	4:H:2001:GBM:H18	2.31	0.45
1:C:313:GLN:HE22	1:C:338:LYS:HD2	1.82	0.45
2:F:24:ASN:O	2:F:28:VAL:HG23	2.17	0.45
2:F:530:MET:CE	2:F:1095:LYS:HG2	2.28	0.45
2:F:892:GLN:H	2:F:892:GLN:HG3	1.46	0.45
2:H:223:ASN:OD1	2:H:223:ASN:N	2.41	0.45
2:H:808:LEU:HG	2:H:812:ILE:HG12	1.99	0.45
1:A:60:PHE:O	1:A:63:LEU:HG	2.17	0.45
2:B:875:GLU:O	2:B:879:ASP:HB2	2.17	0.45
2:B:1246:ARG:HH21	4:B:2001:GBM:H18	1.82	0.45
1:E:60:PHE:O	1:E:63:LEU:HG	2.17	0.45
1:G:170:LYS:O	1:G:173:GLN:HG2	2.17	0.45
1:G:209:MET:HE3	1:G:209:MET:HB3	1.86	0.45
2:H:856:PRO:HD2	2:H:886:LEU:HD21	1.99	0.45
2:H:891:LEU:H	2:H:891:LEU:HD23	1.81	0.45
2:B:1460:LEU:HD13	2:B:1489:LEU:HD23	1.99	0.44
2:D:1369:ILE:HD13	2:D:1375:ILE:HG13	1.99	0.44
1:E:241:GLU:HG3	1:E:259:HIS:HD2	1.82	0.44
2:F:379:VAL:O	2:F:383:THR:OG1	2.35	0.44
2:F:581:SER:O	2:F:585:ILE:HG12	2.17	0.44
2:F:739:TRP:HE1	2:F:768:GLY:N	2.15	0.44
2:H:530:MET:CE	2:H:1095:LYS:HG2	2.28	0.44
2:H:875:GLU:O	2:H:879:ASP:HB2	2.17	0.44
2:H:1355:ASP:OD1	2:H:1356:SER:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:VAL:O	2:B:383:THR:OG1	2.35	0.44
1:C:60:PHE:O	1:C:63:LEU:HG	2.17	0.44
2:D:1246:ARG:HH21	4:D:2001:GBM:H18	1.82	0.44
2:D:1460:LEU:HD13	2:D:1489:LEU:HD23	1.99	0.44
2:F:891:LEU:H	2:F:891:LEU:HD23	1.81	0.44
2:B:24:ASN:O	2:B:28:VAL:HG23	2.17	0.44
2:B:512:TYR:HB2	2:B:1498:ARG:NH2	2.24	0.44
2:B:581:SER:O	2:B:585:ILE:HG12	2.17	0.44
1:C:170:LYS:O	1:C:173:GLN:HG2	2.17	0.44
2:D:402:LEU:O	2:D:1215:ARG:NH1	2.50	0.44
2:H:810:PRO:O	2:H:814:ILE:HG13	2.18	0.44
2:H:1369:ILE:HD13	2:H:1375:ILE:HG13	1.99	0.44
2:B:509:LEU:HD11	2:B:515:GLU:HA	2.00	0.44
2:B:511:LEU:HG	2:B:1424:ILE:HG21	1.98	0.44
2:B:856:PRO:HD2	2:B:886:LEU:HD21	1.99	0.44
2:D:24:ASN:O	2:D:28:VAL:HG23	2.17	0.44
2:D:370:ARG:HG3	2:D:1253:GLU:CD	2.42	0.44
2:F:370:ARG:HG3	2:F:1253:GLU:CD	2.42	0.44
2:F:511:LEU:HG	2:F:1424:ILE:HG21	1.98	0.44
2:H:24:ASN:O	2:H:28:VAL:HG23	2.17	0.44
2:H:370:ARG:HG3	2:H:1253:GLU:CD	2.42	0.44
2:H:509:LEU:HD11	2:H:515:GLU:HA	2.00	0.44
2:H:581:SER:O	2:H:585:ILE:HG12	2.17	0.44
2:B:790:PHE:HB3	2:B:846:GLN:HE21	1.83	0.44
2:D:511:LEU:HG	2:D:1424:ILE:HG21	1.98	0.44
2:D:790:PHE:HB3	2:D:846:GLN:HE21	1.83	0.44
2:F:218:LEU:H	2:F:218:LEU:HG	1.70	0.44
2:H:678:CYS:HB3	2:H:704:PRO:HA	1.99	0.44
2:H:790:PHE:HB3	2:H:846:GLN:HE21	1.83	0.44
2:B:189:VAL:O	2:B:193:ARG:HG2	2.18	0.44
2:B:1154:LEU:HD22	2:B:1168:LEU:HD13	2.00	0.44
2:D:253:LEU:HD12	2:D:253:LEU:HA	1.86	0.44
2:D:810:PRO:O	2:D:814:ILE:HG13	2.18	0.44
2:F:894:LEU:HB2	2:F:895:PRO:HD3	1.99	0.44
1:A:241:GLU:HG3	1:A:259:HIS:HD2	1.82	0.44
2:B:1375:ILE:HD12	2:B:1548:LEU:HB2	2.00	0.44
1:E:169:MET:HB2	1:G:168:PHE:HE1	1.83	0.44
2:F:790:PHE:HB3	2:F:846:GLN:HE21	1.83	0.44
2:F:856:PRO:HD2	2:F:886:LEU:HD21	1.99	0.44
2:F:1039:ASP:OD1	2:F:1039:ASP:N	2.50	0.44
2:D:297:ARG:O	2:D:300:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:297:ARG:O	2:F:300:ILE:HG13	2.18	0.44
1:G:313:GLN:HE22	1:G:338:LYS:HD2	1.82	0.44
2:H:511:LEU:HG	2:H:1424:ILE:HG21	1.98	0.44
2:B:297:ARG:O	2:B:300:ILE:HG13	2.18	0.44
2:F:1246:ARG:HH21	4:F:2001:GBM:H18	1.82	0.44
2:H:1122:LEU:HD12	2:H:1122:LEU:C	2.42	0.44
2:H:1393:PHE:O	2:H:1394:ARG:HG3	2.18	0.44
1:A:168:PHE:HE1	1:G:169:MET:HB2	1.83	0.43
2:B:306:ARG:NH2	4:B:2001:GBM:CL1	2.72	0.43
2:B:891:LEU:HD23	2:B:891:LEU:H	1.81	0.43
2:B:1393:PHE:O	2:B:1394:ARG:HG3	2.18	0.43
2:D:581:SER:O	2:D:585:ILE:HG12	2.17	0.43
2:D:1353:ARG:HH11	2:D:1398:MET:HE3	1.83	0.43
2:F:189:VAL:O	2:F:193:ARG:HG2	2.18	0.43
2:F:400:MET:HA	2:F:400:MET:HE2	2.00	0.43
2:F:509:LEU:HD11	2:F:515:GLU:HA	2.00	0.43
2:H:681:ILE:HD11	2:H:726:THR:HG22	1.99	0.43
2:H:1460:LEU:HD13	2:H:1489:LEU:HD23	1.99	0.43
2:B:1369:ILE:HD13	2:B:1375:ILE:HG13	1.99	0.43
2:D:189:VAL:O	2:D:193:ARG:HG2	2.18	0.43
2:D:891:LEU:HD23	2:D:891:LEU:H	1.81	0.43
2:D:1246:ARG:HA	2:D:1246:ARG:HD3	1.71	0.43
2:F:1393:PHE:O	2:F:1394:ARG:HG3	2.18	0.43
2:F:1460:LEU:HD13	2:F:1489:LEU:HD23	1.99	0.43
2:H:512:TYR:HB2	2:H:1498:ARG:NH2	2.24	0.43
1:A:169:MET:HB2	1:C:168:PHE:HE1	1.83	0.43
1:C:169:MET:HB2	1:E:168:PHE:HE1	1.83	0.43
2:D:681:ILE:HD11	2:D:726:THR:HG22	1.99	0.43
2:F:1201:LEU:HD23	2:F:1201:LEU:HA	1.84	0.43
2:H:79:PHE:CZ	2:H:225:LEU:HD12	2.35	0.43
2:B:681:ILE:HD11	2:B:726:THR:HG22	1.99	0.43
2:B:1246:ARG:HA	2:B:1246:ARG:HD3	1.71	0.43
2:F:1154:LEU:HD22	2:F:1168:LEU:HD13	2.00	0.43
1:G:60:PHE:O	1:G:63:LEU:HG	2.17	0.43
2:H:189:VAL:O	2:H:193:ARG:HG2	2.18	0.43
2:B:1031:ASP:OD2	2:B:1287:TYR:OH	2.25	0.43
2:D:396:TYR:CE2	2:D:1224:GLN:HG3	2.54	0.43
2:D:400:MET:HE2	2:D:400:MET:HA	2.00	0.43
2:D:509:LEU:HD11	2:D:515:GLU:HA	2.00	0.43
2:D:856:PRO:HD2	2:D:886:LEU:HD21	1.99	0.43
2:D:1154:LEU:HD22	2:D:1168:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:810:PRO:O	2:F:814:ILE:HG13	2.18	0.43
2:F:1122:LEU:HD12	2:F:1122:LEU:C	2.42	0.43
1:G:241:GLU:HG3	1:G:259:HIS:HD2	1.82	0.43
2:H:297:ARG:O	2:H:300:ILE:HG13	2.18	0.43
2:H:812:ILE:HD13	2:H:812:ILE:HA	1.84	0.43
2:B:400:MET:HE2	2:B:400:MET:HA	2.00	0.43
2:B:894:LEU:HB2	2:B:895:PRO:HD3	1.99	0.43
1:C:241:GLU:HG3	1:C:259:HIS:HD2	1.82	0.43
2:F:686:PHE:CE2	2:F:730:MET:HB3	2.54	0.43
2:H:1375:ILE:HD12	2:H:1548:LEU:HB2	2.00	0.43
1:C:338:LYS:HB3	1:C:338:LYS:HE3	1.87	0.43
2:D:76:ILE:O	2:D:80:ILE:HG13	2.19	0.43
2:D:512:TYR:HB2	2:D:1498:ARG:NH2	2.24	0.43
2:D:1375:ILE:HD12	2:D:1548:LEU:HB2	2.00	0.43
2:F:681:ILE:HD11	2:F:726:THR:HG22	1.99	0.43
2:F:1347:ILE:HG22	2:F:1350:LEU:HB2	2.01	0.43
2:H:400:MET:HA	2:H:400:MET:HE2	2.00	0.43
4:H:2001:GBM:H20	4:H:2001:GBM:H22	1.75	0.43
2:B:396:TYR:CE2	2:B:1224:GLN:HG3	2.54	0.43
2:B:530:MET:CE	2:B:1095:LYS:HG2	2.28	0.43
2:B:1240:PHE:HD1	2:B:1240:PHE:HA	1.66	0.43
2:D:894:LEU:HB2	2:D:895:PRO:HD3	1.99	0.43
2:D:1124:ARG:O	2:D:1128:ASP:HB2	2.19	0.43
4:D:2001:GBM:H20	4:D:2001:GBM:H22	1.75	0.43
2:F:150:LYS:HB3	2:F:176:VAL:HG22	2.01	0.43
2:F:869:MET:HE3	2:F:869:MET:HB3	1.87	0.43
2:H:894:LEU:HB2	2:H:895:PRO:HD3	1.99	0.43
2:B:511:LEU:HD23	2:B:1426:LEU:HD21	2.01	0.43
2:B:1124:ARG:O	2:B:1128:ASP:HB2	2.19	0.43
1:C:332:LYS:HD3	1:C:335:ASN:OD1	2.19	0.43
2:D:1355:ASP:OD1	2:D:1356:SER:N	2.50	0.43
2:F:37:VAL:HG13	2:F:41:PHE:CE2	2.54	0.43
2:F:1355:ASP:OD1	2:F:1356:SER:N	2.50	0.43
2:B:511:LEU:HD13	2:B:511:LEU:HA	1.85	0.43
2:B:686:PHE:CE2	2:B:730:MET:HB3	2.54	0.43
2:B:810:PRO:O	2:B:814:ILE:HG13	2.18	0.43
2:D:530:MET:CE	2:D:1095:LYS:HG2	2.28	0.43
2:D:1475:ILE:HD12	2:D:1482:PHE:HE2	1.84	0.43
2:F:76:ILE:O	2:F:80:ILE:HG13	2.19	0.43
2:H:37:VAL:HG13	2:H:41:PHE:CE2	2.54	0.43
2:H:1039:ASP:OD1	2:H:1039:ASP:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1124:ARG:O	2:H:1128:ASP:HB2	2.19	0.43
2:H:1246:ARG:HH21	4:H:2001:GBM:H18	1.82	0.43
2:H:1347:ILE:HG22	2:H:1350:LEU:HB2	2.01	0.43
2:H:1353:ARG:HH11	2:H:1398:MET:HE3	1.83	0.43
2:B:76:ILE:O	2:B:80:ILE:HG13	2.19	0.42
2:D:598:ARG:HD3	2:D:598:ARG:C	2.44	0.42
2:F:396:TYR:CE2	2:F:1224:GLN:HG3	2.54	0.42
1:A:332:LYS:HD3	1:A:335:ASN:OD1	2.19	0.42
2:B:514:TRP:HA	2:B:517:ILE:HD13	2.01	0.42
2:B:1353:ARG:HH11	2:B:1398:MET:HE3	1.83	0.42
2:D:37:VAL:HG13	2:D:41:PHE:CE2	2.54	0.42
2:D:218:LEU:H	2:D:218:LEU:HG	1.70	0.42
2:F:306:ARG:NH2	4:F:2001:GBM:CL1	2.72	0.42
2:F:1240:PHE:HD1	2:F:1240:PHE:HA	1.66	0.42
1:G:332:LYS:HD3	1:G:335:ASN:OD1	2.19	0.42
2:H:76:ILE:O	2:H:80:ILE:HG13	2.19	0.42
2:H:528:LYS:HE3	2:H:528:LYS:HB3	1.84	0.42
2:H:869:MET:HE3	2:H:869:MET:HB3	1.87	0.42
2:H:1475:ILE:HD12	2:H:1482:PHE:HE2	1.84	0.42
2:B:37:VAL:HG13	2:B:41:PHE:CE2	2.54	0.42
2:B:1200:LEU:HD13	2:B:1230:TYR:HB3	2.01	0.42
2:D:150:LYS:HB3	2:D:176:VAL:HG22	2.01	0.42
2:D:1393:PHE:O	2:D:1394:ARG:HG3	2.18	0.42
2:F:402:LEU:O	2:F:1215:ARG:NH1	2.50	0.42
2:H:511:LEU:HD23	2:H:1426:LEU:HD21	2.01	0.42
2:H:1154:LEU:HD22	2:H:1168:LEU:HD13	2.00	0.42
1:A:79:PHE:HD1	1:A:79:PHE:HA	1.74	0.42
2:B:1437:ARG:HG3	2:B:1471:LEU:O	2.20	0.42
2:B:1452:TRP:CE3	2:B:1461:LYS:HE3	2.55	0.42
2:D:1108:ALA:HB3	2:D:1113:PHE:CE2	2.55	0.42
2:D:1365:VAL:HG22	2:D:1557:ILE:HG13	2.01	0.42
1:E:332:LYS:HD3	1:E:335:ASN:OD1	2.19	0.42
2:F:1108:ALA:HB3	2:F:1113:PHE:CE2	2.55	0.42
2:H:708:LEU:HB3	2:H:897:ALA:HA	2.02	0.42
2:B:219:GLN:HG2	2:B:378:TYR:OH	2.20	0.42
2:D:1200:LEU:HD13	2:D:1230:TYR:HB3	2.01	0.42
2:F:1353:ARG:HH11	2:F:1398:MET:HE3	1.83	0.42
2:F:1365:VAL:HG22	2:F:1557:ILE:HG13	2.01	0.42
2:F:1375:ILE:HD12	2:F:1548:LEU:HB2	2.00	0.42
1:G:261:ILE:H	1:G:261:ILE:HG13	1.61	0.42
2:H:402:LEU:O	2:H:1215:ARG:NH1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:719:LYS:HB3	2:H:887:VAL:HG11	2.01	0.42
2:H:1108:ALA:HB3	2:H:1113:PHE:CE2	2.55	0.42
1:A:145:ALA:HA	1:A:148:ILE:HG22	2.02	0.42
2:B:719:LYS:HB3	2:B:887:VAL:HG11	2.01	0.42
2:D:514:TRP:HA	2:D:517:ILE:HD13	2.01	0.42
2:D:686:PHE:CE2	2:D:730:MET:HB3	2.54	0.42
2:D:1031:ASP:OD2	2:D:1287:TYR:OH	2.25	0.42
2:F:1124:ARG:O	2:F:1128:ASP:HB2	2.19	0.42
2:B:150:LYS:HB3	2:B:176:VAL:HG22	2.01	0.42
2:B:1347:ILE:HG22	2:B:1350:LEU:HB2	2.01	0.42
1:C:61:THR:O	1:C:64:VAL:HG22	2.20	0.42
1:C:86:PHE:HA	1:C:89:VAL:HG12	2.02	0.42
1:C:286:ILE:HD12	1:C:301:ARG:HG2	2.02	0.42
1:E:61:THR:O	1:E:64:VAL:HG22	2.20	0.42
1:E:86:PHE:HA	1:E:89:VAL:HG12	2.02	0.42
2:F:219:GLN:HG2	2:F:378:TYR:OH	2.20	0.42
2:F:708:LEU:HB3	2:F:897:ALA:HA	2.02	0.42
2:F:852:PHE:CD1	2:F:885:VAL:HB	2.55	0.42
2:H:150:LYS:HB3	2:H:176:VAL:HG22	2.01	0.42
2:H:686:PHE:CE2	2:H:730:MET:HB3	2.54	0.42
2:H:1132:ILE:HA	2:H:1136:ILE:HD13	2.02	0.42
2:B:1201:LEU:HD23	2:B:1201:LEU:HA	1.84	0.42
1:E:188:VAL:HG12	1:E:310:LEU:HD11	2.02	0.42
1:E:286:ILE:HD12	1:E:301:ARG:HG2	2.02	0.42
1:E:286:ILE:HG23	1:E:301:ARG:HG2	2.02	0.42
2:F:598:ARG:HD3	2:F:598:ARG:C	2.44	0.42
2:F:1200:LEU:HD13	2:F:1230:TYR:HB3	2.01	0.42
1:G:158:MET:O	1:G:162:ILE:HG22	2.20	0.42
1:G:188:VAL:HG12	1:G:310:LEU:HD11	2.02	0.42
1:G:286:ILE:HG23	1:G:301:ARG:HG2	2.02	0.42
2:H:396:TYR:CE2	2:H:1224:GLN:HG3	2.54	0.42
2:H:514:TRP:HA	2:H:517:ILE:HD13	2.01	0.42
2:H:1316:HIS:HA	2:H:1319:LEU:HD12	2.02	0.42
1:A:220:VAL:HB	1:A:233:LEU:HG	2.02	0.42
2:B:598:ARG:HD3	2:B:598:ARG:C	2.44	0.42
2:B:1127:SER:O	2:B:1130:ASN:N	2.53	0.42
1:C:243:GLY:O	1:C:244:VAL:C	2.63	0.42
2:D:219:GLN:HG2	2:D:378:TYR:OH	2.20	0.42
2:D:1039:ASP:OD1	2:D:1039:ASP:N	2.50	0.42
2:D:1347:ILE:HG22	2:D:1350:LEU:HB2	2.01	0.42
2:F:1132:ILE:HA	2:F:1136:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1475:ILE:HD12	2:F:1482:PHE:HE2	1.84	0.42
2:H:1404:ILE:HG21	2:H:1407:GLY:HA2	2.02	0.42
2:H:1437:ARG:HG3	2:H:1471:LEU:O	2.20	0.42
2:H:1441:ASP:OD2	2:H:1445:LYS:N	2.53	0.42
2:D:1441:ASP:OD2	2:D:1445:LYS:N	2.53	0.41
2:F:511:LEU:HD23	2:F:1426:LEU:HD21	2.01	0.41
1:G:209:MET:HB2	1:G:292:GLU:OE2	2.20	0.41
2:H:598:ARG:HD3	2:H:598:ARG:C	2.44	0.41
2:H:710:MET:HG2	2:H:897:ALA:HB2	2.02	0.41
2:H:1200:LEU:HD13	2:H:1230:TYR:HB3	2.01	0.41
2:H:1240:PHE:HD1	2:H:1240:PHE:HA	1.66	0.41
1:A:243:GLY:O	1:A:244:VAL:C	2.63	0.41
2:B:710:MET:HG2	2:B:897:ALA:HB2	2.02	0.41
2:B:877:LEU:HB3	2:B:884:VAL:HG21	2.02	0.41
2:B:1365:VAL:HG22	2:B:1557:ILE:HG13	2.01	0.41
1:C:145:ALA:HA	1:C:148:ILE:HG22	2.02	0.41
2:D:1437:ARG:HG3	2:D:1471:LEU:O	2.20	0.41
2:F:1316:HIS:HA	2:F:1319:LEU:HD12	2.02	0.41
2:H:817:HIS:O	2:H:821:THR:OG1	2.38	0.41
1:A:86:PHE:HA	1:A:89:VAL:HG12	2.02	0.41
1:A:241:GLU:HB2	1:A:258:TYR:O	2.21	0.41
2:B:817:HIS:O	2:B:821:THR:OG1	2.38	0.41
2:B:1425:ILE:HD13	2:B:1492:LEU:HD12	2.02	0.41
2:B:1475:ILE:HD12	2:B:1482:PHE:HE2	1.84	0.41
2:D:511:LEU:HD23	2:D:1426:LEU:HD21	2.01	0.41
2:D:1132:ILE:HA	2:D:1136:ILE:HD13	2.02	0.41
2:F:526:ARG:NH1	2:F:1098:HIS:ND1	2.68	0.41
2:F:1441:ASP:OD2	2:F:1445:LYS:N	2.53	0.41
1:G:61:THR:O	1:G:64:VAL:HG22	2.20	0.41
1:G:145:ALA:HA	1:G:148:ILE:HG22	2.02	0.41
2:H:852:PHE:CD1	2:H:885:VAL:HB	2.55	0.41
2:H:1452:TRP:CE3	2:H:1461:LYS:HE3	2.55	0.41
2:B:869:MET:HE3	2:B:869:MET:HB3	1.87	0.41
2:B:1108:ALA:HB3	2:B:1113:PHE:CE2	2.55	0.41
1:C:209:MET:HE3	1:C:209:MET:HB3	1.86	0.41
2:D:710:MET:HG2	2:D:897:ALA:HB2	2.02	0.41
2:D:1127:SER:O	2:D:1130:ASN:N	2.53	0.41
1:E:158:MET:O	1:E:162:ILE:HG22	2.20	0.41
1:E:209:MET:HB2	1:E:292:GLU:OE2	2.20	0.41
2:F:530:MET:HE3	2:F:1095:LYS:HG3	1.97	0.41
2:F:710:MET:HG2	2:F:897:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:812:ILE:HD13	2:F:812:ILE:HA	1.84	0.41
2:F:877:LEU:HB3	2:F:884:VAL:HG21	2.02	0.41
2:F:1239:LEU:O	2:F:1242:THR:HG22	2.21	0.41
2:H:1239:LEU:O	2:H:1242:THR:HG22	2.21	0.41
1:A:158:MET:O	1:A:162:ILE:HG22	2.20	0.41
1:A:261:ILE:H	1:A:261:ILE:HG13	1.61	0.41
2:B:1355:ASP:OD1	2:B:1356:SER:N	2.50	0.41
2:B:1441:ASP:OD2	2:B:1445:LYS:N	2.53	0.41
2:D:719:LYS:HB3	2:D:887:VAL:HG11	2.01	0.41
2:D:852:PHE:CD1	2:D:885:VAL:HB	2.55	0.41
2:F:216:ARG:HD2	2:F:251:GLY:N	2.35	0.41
2:F:1452:TRP:CE3	2:F:1461:LYS:HE3	2.55	0.41
1:G:86:PHE:HA	1:G:89:VAL:HG12	2.02	0.41
1:G:125:ILE:HD12	1:G:125:ILE:HA	1.95	0.41
2:H:1127:SER:O	2:H:1130:ASN:N	2.53	0.41
2:H:1425:ILE:HD13	2:H:1492:LEU:HD12	2.02	0.41
1:A:60:PHE:HA	1:A:63:LEU:HD23	2.03	0.41
2:B:903:MET:SD	2:B:908:ILE:HG12	2.60	0.41
2:B:1404:ILE:HG21	2:B:1407:GLY:HA2	2.02	0.41
1:C:60:PHE:HA	1:C:63:LEU:HD23	2.03	0.41
1:C:75:PHE:HB3	1:C:163:MET:SD	2.61	0.41
1:C:209:MET:HB2	1:C:292:GLU:OE2	2.20	0.41
2:D:526:ARG:NH1	2:D:1098:HIS:ND1	2.68	0.41
2:D:1452:TRP:CE3	2:D:1461:LYS:HE3	2.55	0.41
2:F:1437:ARG:HG3	2:F:1471:LEU:O	2.20	0.41
2:H:1060:ASP:OD1	2:H:1060:ASP:N	2.53	0.41
1:A:75:PHE:HB3	1:A:163:MET:SD	2.61	0.41
2:B:104:LEU:O	2:B:108:MET:HG2	2.21	0.41
1:C:241:GLU:HB2	1:C:258:TYR:O	2.21	0.41
1:C:286:ILE:HG23	1:C:301:ARG:HG2	2.02	0.41
2:D:1425:ILE:HD13	2:D:1492:LEU:HD12	2.02	0.41
1:E:60:PHE:HA	1:E:63:LEU:HD23	2.03	0.41
1:E:145:ALA:HA	1:E:148:ILE:HG22	2.02	0.41
1:E:241:GLU:HB2	1:E:258:TYR:O	2.21	0.41
2:H:104:LEU:O	2:H:108:MET:HG2	2.21	0.41
2:H:219:GLN:HG2	2:H:378:TYR:OH	2.20	0.41
1:A:188:VAL:HG12	1:A:310:LEU:HD11	2.02	0.41
1:A:338:LYS:HE3	1:A:338:LYS:HB3	1.87	0.41
2:B:708:LEU:HB3	2:B:897:ALA:HA	2.02	0.41
2:B:812:ILE:HD13	2:B:812:ILE:HA	1.84	0.41
2:B:1062:SER:O	2:B:1066:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1132:ILE:HA	2:B:1136:ILE:HD13	2.02	0.41
2:D:104:LEU:O	2:D:108:MET:HG2	2.21	0.41
1:E:75:PHE:HB3	1:E:163:MET:SD	2.61	0.41
2:F:253:LEU:HD12	2:F:253:LEU:HA	1.86	0.41
2:F:719:LYS:HB3	2:F:887:VAL:HG11	2.01	0.41
2:F:1404:ILE:HG21	2:F:1407:GLY:HA2	2.02	0.41
1:G:220:VAL:HB	1:G:233:LEU:HG	2.02	0.41
1:G:243:GLY:O	1:G:244:VAL:C	2.63	0.41
1:G:297:THR:O	1:G:297:THR:OG1	2.37	0.41
2:H:526:ARG:NH1	2:H:1098:HIS:ND1	2.68	0.41
2:H:903:MET:SD	2:H:908:ILE:HG12	2.60	0.41
1:A:61:THR:O	1:A:64:VAL:HG22	2.20	0.41
2:B:253:LEU:HD12	2:B:253:LEU:HA	1.86	0.41
2:B:309:ALA:O	2:B:369:GLN:HG3	2.21	0.41
2:B:852:PHE:CD1	2:B:885:VAL:HB	2.55	0.41
2:D:306:ARG:NH2	4:D:2001:GBM:CL1	2.72	0.41
2:D:708:LEU:HB3	2:D:897:ALA:HA	2.02	0.41
2:D:795:ASN:O	2:D:799:TYR:HB3	2.21	0.41
2:D:903:MET:SD	2:D:908:ILE:HG12	2.60	0.41
2:D:1394:ARG:HG2	2:D:1410:ILE:HG21	2.03	0.41
2:F:514:TRP:HA	2:F:517:ILE:HD13	2.01	0.41
2:F:795:ASN:HB3	2:F:798:ARG:HB3	2.03	0.41
2:F:1127:SER:O	2:F:1130:ASN:N	2.53	0.41
2:F:1246:ARG:HA	2:F:1246:ARG:HD3	1.71	0.41
1:G:286:ILE:HD12	1:G:301:ARG:HG2	2.02	0.41
2:H:126:ASN:HA	2:H:129:THR:HG22	2.03	0.41
2:H:1062:SER:O	2:H:1066:MET:HG2	2.21	0.41
2:H:1152:SER:O	2:H:1156:VAL:HG23	2.21	0.41
1:A:286:ILE:HG23	1:A:301:ARG:HG2	2.02	0.41
2:B:530:MET:HE3	2:B:1095:LYS:HG3	1.97	0.41
2:B:795:ASN:O	2:B:799:TYR:HB3	2.21	0.41
2:B:1239:LEU:O	2:B:1242:THR:HG22	2.21	0.41
1:C:181:LEU:HD23	1:C:287:LEU:HD21	2.03	0.41
2:D:126:ASN:HA	2:D:129:THR:HG22	2.03	0.41
2:D:216:ARG:HD2	2:D:251:GLY:N	2.35	0.41
2:D:881:LYS:HA	2:D:881:LYS:HD3	1.89	0.41
1:E:243:GLY:O	1:E:244:VAL:C	2.63	0.41
2:F:104:LEU:O	2:F:108:MET:HG2	2.21	0.41
2:F:795:ASN:O	2:F:799:TYR:HB3	2.21	0.41
2:F:1106:ILE:HD13	2:F:1106:ILE:HA	1.78	0.41
2:F:1152:SER:O	2:F:1156:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:471:ALA:HB3	2:H:472:PRO:HD3	2.03	0.41
2:H:576:ALA:O	2:H:579:SER:OG	2.33	0.41
1:A:125:ILE:HD12	1:A:125:ILE:HA	1.95	0.40
2:B:1060:ASP:OD1	2:B:1060:ASP:N	2.53	0.40
2:B:1363:LYS:HE3	2:B:1364:HIS:CE1	2.57	0.40
1:C:158:MET:O	1:C:162:ILE:HG22	2.20	0.40
1:C:188:VAL:HG12	1:C:310:LEU:HD11	2.02	0.40
2:D:1106:ILE:HA	2:D:1106:ILE:HD13	1.78	0.40
2:D:1239:LEU:O	2:D:1242:THR:HG22	2.21	0.40
2:D:1363:LYS:HE3	2:D:1364:HIS:CE1	2.57	0.40
2:D:1404:ILE:HG21	2:D:1407:GLY:HA2	2.02	0.40
1:E:181:LEU:HD23	1:E:287:LEU:HD21	2.03	0.40
1:E:183:PHE:CD2	1:E:202:VAL:HG12	2.57	0.40
1:E:189:ILE:HD11	1:E:311:TRP:CE2	2.56	0.40
2:F:903:MET:SD	2:F:908:ILE:HG12	2.60	0.40
2:F:1062:SER:O	2:F:1066:MET:HG2	2.21	0.40
2:F:1394:ARG:HG2	2:F:1410:ILE:HG21	2.03	0.40
1:G:75:PHE:HB3	1:G:163:MET:SD	2.61	0.40
1:G:238:ILE:HA	1:G:239:PRO:HD3	1.96	0.40
2:H:681:ILE:HB	2:H:701:ILE:HG23	2.03	0.40
2:H:795:ASN:O	2:H:799:TYR:HB3	2.21	0.40
2:H:1365:VAL:HG22	2:H:1557:ILE:HG13	2.01	0.40
1:A:181:LEU:HD23	1:A:287:LEU:HD21	2.03	0.40
1:C:220:VAL:HB	1:C:233:LEU:HG	2.02	0.40
1:C:284:ILE:HA	1:C:302:THR:O	2.21	0.40
1:E:220:VAL:HB	1:E:233:LEU:HG	2.02	0.40
2:F:478:ALA:O	2:F:481:LEU:HB3	2.21	0.40
2:F:1255:ILE:HD13	2:F:1255:ILE:HA	1.91	0.40
2:F:1363:LYS:HE3	2:F:1364:HIS:CE1	2.57	0.40
2:F:1425:ILE:HD13	2:F:1492:LEU:HD12	2.02	0.40
1:G:60:PHE:HA	1:G:63:LEU:HD23	2.03	0.40
1:G:79:PHE:HD1	1:G:79:PHE:HA	1.74	0.40
2:H:45:PRO:O	2:H:49:ILE:HG13	2.22	0.40
2:H:699:ILE:HG12	2:H:908:ILE:HG13	2.03	0.40
2:H:1063:VAL:O	2:H:1067:VAL:HG23	2.21	0.40
2:H:1405:ILE:HD13	2:H:1422:LEU:HD21	2.04	0.40
1:A:189:ILE:HD11	1:A:311:TRP:CE2	2.56	0.40
1:A:209:MET:HB2	1:A:292:GLU:OE2	2.20	0.40
1:A:286:ILE:HD12	1:A:301:ARG:HG2	2.02	0.40
2:B:45:PRO:O	2:B:49:ILE:HG13	2.22	0.40
2:B:526:ARG:NH1	2:B:1098:HIS:ND1	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:681:ILE:HB	2:B:701:ILE:HG23	2.03	0.40
2:B:1405:ILE:HD13	2:B:1422:LEU:HD21	2.04	0.40
2:D:45:PRO:O	2:D:49:ILE:HG13	2.22	0.40
2:D:471:ALA:HB3	2:D:472:PRO:HD3	2.03	0.40
2:F:817:HIS:O	2:F:821:THR:OG1	2.38	0.40
1:G:241:GLU:HB2	1:G:258:TYR:O	2.21	0.40
2:B:1404:ILE:CG2	2:B:1408:ILE:N	2.84	0.40
2:D:576:ALA:O	2:D:579:SER:OG	2.33	0.40
2:F:156:LYS:HA	2:F:156:LYS:HD3	1.89	0.40
2:F:471:ALA:HB3	2:F:472:PRO:HD3	2.03	0.40
2:H:216:ARG:HD2	2:H:251:GLY:N	2.35	0.40
2:H:795:ASN:HB3	2:H:798:ARG:HB3	2.03	0.40
2:H:877:LEU:HB3	2:H:884:VAL:HG21	2.02	0.40
2:B:1152:SER:O	2:B:1156:VAL:HG23	2.21	0.40
2:B:1316:HIS:HA	2:B:1319:LEU:HD12	2.02	0.40
2:D:309:ALA:O	2:D:369:GLN:HG3	2.21	0.40
2:D:817:HIS:O	2:D:821:THR:OG1	2.38	0.40
2:D:1152:SER:O	2:D:1156:VAL:HG23	2.21	0.40
2:D:1251:ARG:HB2	2:D:1251:ARG:NH1	2.36	0.40
2:F:1063:VAL:O	2:F:1067:VAL:HG23	2.21	0.40
1:G:189:ILE:HD11	1:G:311:TRP:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	118/339 (35%)	104 (88%)	14 (12%)	5 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	253/339 (75%)	219 (87%)	34 (13%)	4	16
1	G	253/339 (75%)	219 (87%)	34 (13%)	4	16
2	B	871/1371 (64%)	817 (94%)	54 (6%)	16	38
2	D	1102/1371 (80%)	1029 (93%)	73 (7%)	15	37
2	F	1102/1371 (80%)	1029 (93%)	73 (7%)	15	37
2	H	297/1371 (22%)	276 (93%)	21 (7%)	13	35
All	All	3996/6501 (62%)	3693 (92%)	303 (8%)	14	33

All (303) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	318	LEU
2	B	327	LEU
2	B	357	VAL
2	B	374	GLN
2	B	383	THR
2	B	391	ILE
2	B	399	ILE
2	B	420	LEU
2	B	428	LEU
2	B	430	TRP
2	B	432	PHE
2	B	458	VAL
2	B	467	ILE
2	B	470	LEU
2	B	511	LEU
2	B	512	TYR
2	B	598	ARG
2	B	682	ILE
2	B	689	THR
2	B	696	LEU
2	B	701	ILE
2	B	708	LEU
2	B	737	VAL
2	B	770	VAL
2	B	812	ILE
2	B	829	ASN
2	B	892	GLN
2	B	1001	CYS
2	B	1106	ILE

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Mol	Chain	Res	Type
2	B	1122	LEU
2	B	1129	CYS
2	B	1136	ILE
2	B	1157	ILE
2	B	1168	LEU
2	B	1178	ILE
2	B	1195	THR
2	B	1204	PHE
2	B	1238	SER
2	B	1240	PHE
2	B	1246	ARG
2	B	1251	ARG
2	B	1254	TYR
2	B	1268	ILE
2	B	1276	LEU
2	B	1296	ASN
2	B	1318	LEU
2	B	1383	SER
2	B	1394	ARG
2	B	1396	VAL
2	B	1410	ILE
2	B	1432	PHE
2	B	1488	GLN
2	B	1522	LYS
2	B	1524	VAL
1	C	122	LEU
1	C	152	GLN
1	C	181	LEU
1	C	182	ILE
1	C	261	ILE
1	C	287	LEU
1	C	290	VAL
1	C	294	THR
1	C	297	THR
1	C	298	THR
1	C	310	LEU
1	C	323	ASP
1	C	345	THR
1	C	349	LEU
2	D	37	VAL
2	D	42	ILE
2	D	72	ASN

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Mol	Chain	Res	Type
2	D	119	THR
2	D	121	VAL
2	D	123	TYR
2	D	167	LEU
2	D	196	ILE
2	D	204	VAL
2	D	218	LEU
2	D	222	VAL
2	D	223	ASN
2	D	253	LEU
2	D	318	LEU
2	D	327	LEU
2	D	357	VAL
2	D	374	GLN
2	D	383	THR
2	D	391	ILE
2	D	399	ILE
2	D	420	LEU
2	D	428	LEU
2	D	430	TRP
2	D	432	PHE
2	D	458	VAL
2	D	467	ILE
2	D	470	LEU
2	D	511	LEU
2	D	512	TYR
2	D	598	ARG
2	D	682	ILE
2	D	689	THR
2	D	696	LEU
2	D	701	ILE
2	D	708	LEU
2	D	737	VAL
2	D	770	VAL
2	D	812	ILE
2	D	829	ASN
2	D	892	GLN
2	D	1001	CYS
2	D	1106	ILE
2	D	1122	LEU
2	D	1129	CYS
2	D	1136	ILE

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Mol	Chain	Res	Type
2	D	1157	ILE
2	D	1168	LEU
2	D	1178	ILE
2	D	1195	THR
2	D	1204	PHE
2	D	1238	SER
2	D	1240	PHE
2	D	1246	ARG
2	D	1251	ARG
2	D	1254	TYR
2	D	1268	ILE
2	D	1276	LEU
2	D	1296	ASN
2	D	1318	LEU
2	D	1383	SER
2	D	1394	ARG
2	D	1396	VAL
2	D	1410	ILE
2	D	1432	PHE
2	D	1488	GLN
2	D	1522	LYS
2	D	1524	VAL
2	D	1536	ILE
2	D	1550	MET
2	D	1551	VAL
2	D	1557	ILE
2	D	1561	ASP
2	D	1566	LEU
1	E	36	VAL
1	E	60	PHE
1	E	63	LEU
1	E	64	VAL
1	E	71	THR
1	E	81	CYS
1	E	88	MET
1	E	90	TRP
1	E	108	VAL
1	E	111	VAL
1	E	122	LEU
1	E	133	PHE
1	E	152	GLN
1	E	181	LEU

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Mol	Chain	Res	Type
1	E	182	ILE
1	E	190	THR
1	E	204	ASP
1	E	205	LEU
1	E	219	VAL
1	E	236	VAL
1	E	238	ILE
1	E	249	ILE
1	E	252	VAL
1	E	256	ILE
1	E	261	ILE
1	E	287	LEU
1	E	290	VAL
1	E	294	THR
1	E	297	THR
1	E	298	THR
1	E	310	LEU
1	E	323	ASP
1	E	345	THR
1	E	349	LEU
2	F	37	VAL
2	F	42	ILE
2	F	72	ASN
2	F	119	THR
2	F	121	VAL
2	F	123	TYR
2	F	167	LEU
2	F	196	ILE
2	F	204	VAL
2	F	218	LEU
2	F	222	VAL
2	F	223	ASN
2	F	253	LEU
2	F	318	LEU
2	F	327	LEU
2	F	357	VAL
2	F	374	GLN
2	F	383	THR
2	F	391	ILE
2	F	399	ILE
2	F	420	LEU
2	F	428	LEU

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Mol	Chain	Res	Type
2	F	430	TRP
2	F	432	PHE
2	F	458	VAL
2	F	467	ILE
2	F	470	LEU
2	F	511	LEU
2	F	512	TYR
2	F	598	ARG
2	F	682	ILE
2	F	689	THR
2	F	696	LEU
2	F	701	ILE
2	F	708	LEU
2	F	737	VAL
2	F	770	VAL
2	F	812	ILE
2	F	829	ASN
2	F	892	GLN
2	F	1001	CYS
2	F	1106	ILE
2	F	1122	LEU
2	F	1129	CYS
2	F	1136	ILE
2	F	1157	ILE
2	F	1168	LEU
2	F	1178	ILE
2	F	1195	THR
2	F	1204	PHE
2	F	1238	SER
2	F	1240	PHE
2	F	1246	ARG
2	F	1251	ARG
2	F	1254	TYR
2	F	1268	ILE
2	F	1276	LEU
2	F	1296	ASN
2	F	1318	LEU
2	F	1383	SER
2	F	1394	ARG
2	F	1396	VAL
2	F	1410	ILE
2	F	1432	PHE

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Mol	Chain	Res	Type
2	F	1488	GLN
2	F	1522	LYS
2	F	1524	VAL
2	F	1536	ILE
2	F	1550	MET
2	F	1551	VAL
2	F	1557	ILE
2	F	1561	ASP
2	F	1566	LEU
1	G	36	VAL
1	G	60	PHE
1	G	63	LEU
1	G	64	VAL
1	G	71	THR
1	G	81	CYS
1	G	88	MET
1	G	90	TRP
1	G	108	VAL
1	G	111	VAL
1	G	122	LEU
1	G	133	PHE
1	G	152	GLN
1	G	181	LEU
1	G	182	ILE
1	G	190	THR
1	G	204	ASP
1	G	205	LEU
1	G	219	VAL
1	G	236	VAL
1	G	238	ILE
1	G	249	ILE
1	G	252	VAL
1	G	256	ILE
1	G	261	ILE
1	G	287	LEU
1	G	290	VAL
1	G	294	THR
1	G	297	THR
1	G	298	THR
1	G	310	LEU
1	G	323	ASP
1	G	345	THR

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Mol	Chain	Res	Type
1	G	349	LEU
2	H	37	VAL
2	H	42	ILE
2	H	72	ASN
2	H	119	THR
2	H	121	VAL
2	H	123	TYR
2	H	167	LEU
2	H	1383	SER
2	H	1394	ARG
2	H	1396	VAL
2	H	1410	ILE
2	H	1432	PHE
2	H	1488	GLN
2	H	1522	LYS
2	H	1524	VAL
2	H	1536	ILE
2	H	1550	MET
2	H	1551	VAL
2	H	1557	ILE
2	H	1561	ASP
2	H	1566	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	326	HIS
2	B	491	HIS
2	B	834	GLN
2	B	1020	GLN
2	B	1135	HIS
2	B	1190	GLN
2	B	1518	ASN
2	B	1521	GLN
2	D	219	GLN
2	D	262	ASN
2	D	326	HIS
2	D	491	HIS
2	D	834	GLN
2	D	1020	GLN
2	D	1135	HIS
2	D	1190	GLN

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Mol	Chain	Res	Type
2	D	1518	ASN
2	D	1521	GLN
1	E	46	HIS
1	E	48	ASN
1	E	128	GLN
1	E	216	HIS
1	E	234	HIS
1	E	259	HIS
2	F	219	GLN
2	F	326	HIS
2	F	491	HIS
2	F	834	GLN
2	F	1020	GLN
2	F	1135	HIS
2	F	1190	GLN
2	F	1518	ASN
2	F	1521	GLN
1	G	46	HIS
1	G	48	ASN
1	G	128	GLN
1	G	216	HIS
1	G	234	HIS
1	G	259	HIS
2	H	1518	ASN
2	H	1521	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AGS	H	2002	-	32,33,33	2.06	8 (25%)	45,52,52	1.85	9 (20%)
3	AGS	F	2002	-	32,33,33	2.06	8 (25%)	45,52,52	1.85	9 (20%)
3	AGS	E	401	-	32,33,33	2.04	6 (18%)	45,52,52	1.84	9 (20%)
3	AGS	A	401	-	32,33,33	2.04	6 (18%)	45,52,52	1.84	9 (20%)
3	AGS	B	2002	-	32,33,33	2.06	8 (25%)	45,52,52	1.85	9 (20%)
4	GBM	D	2001	-	35,35,35	2.03	4 (11%)	48,48,48	1.88	7 (14%)
4	GBM	H	2001	-	35,35,35	2.03	4 (11%)	48,48,48	1.88	7 (14%)
3	AGS	C	401	-	32,33,33	2.04	6 (18%)	45,52,52	1.84	9 (20%)
4	GBM	F	2001	-	35,35,35	2.03	4 (11%)	48,48,48	1.88	7 (14%)
3	AGS	D	2002	-	32,33,33	2.06	8 (25%)	45,52,52	1.85	9 (20%)
4	GBM	B	2001	-	35,35,35	2.03	4 (11%)	48,48,48	1.88	7 (14%)
3	AGS	G	401	-	32,33,33	2.04	6 (18%)	45,52,52	1.84	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	H	2002	-	-	2/21/38/38	0/3/3/3
3	AGS	F	2002	-	-	2/21/38/38	0/3/3/3
3	AGS	E	401	-	-	5/21/38/38	0/3/3/3
3	AGS	A	401	-	-	5/21/38/38	0/3/3/3
3	AGS	B	2002	-	-	2/21/38/38	0/3/3/3
4	GBM	D	2001	-	-	8/27/35/35	0/3/3/3
4	GBM	H	2001	-	-	8/27/35/35	0/3/3/3
3	AGS	C	401	-	-	5/21/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GBM	F	2001	-	-	8/27/35/35	0/3/3/3
3	AGS	D	2002	-	-	2/21/38/38	0/3/3/3
4	GBM	B	2001	-	-	8/27/35/35	0/3/3/3
3	AGS	G	401	-	-	5/21/38/38	0/3/3/3

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2001	GBM	C18-S2	-10.15	1.60	1.76
4	D	2001	GBM	C18-S2	-10.15	1.60	1.76
4	F	2001	GBM	C18-S2	-10.15	1.60	1.76
4	H	2001	GBM	C18-S2	-10.15	1.60	1.76
3	A	401	AGS	PG-S1G	7.97	2.08	1.90
3	C	401	AGS	PG-S1G	7.97	2.08	1.90
3	E	401	AGS	PG-S1G	7.97	2.08	1.90
3	G	401	AGS	PG-S1G	7.97	2.08	1.90
3	B	2002	AGS	PG-S1G	7.97	2.08	1.90
3	D	2002	AGS	PG-S1G	7.97	2.08	1.90
3	F	2002	AGS	PG-S1G	7.97	2.08	1.90
3	H	2002	AGS	PG-S1G	7.97	2.08	1.90
4	B	2001	GBM	C27-C28	4.77	1.49	1.40
4	D	2001	GBM	C27-C28	4.77	1.49	1.40
4	F	2001	GBM	C27-C28	4.77	1.49	1.40
4	H	2001	GBM	C27-C28	4.77	1.49	1.40
3	A	401	AGS	C5-C4	4.75	1.47	1.39
3	C	401	AGS	C5-C4	4.75	1.47	1.39
3	E	401	AGS	C5-C4	4.75	1.47	1.39
3	G	401	AGS	C5-C4	4.75	1.47	1.39
3	B	2002	AGS	C5-C4	4.70	1.47	1.39
3	D	2002	AGS	C5-C4	4.70	1.47	1.39
3	F	2002	AGS	C5-C4	4.70	1.47	1.39
3	H	2002	AGS	C5-C4	4.70	1.47	1.39
3	B	2002	AGS	C5-C6	2.74	1.48	1.41
3	D	2002	AGS	C5-C6	2.74	1.48	1.41
3	F	2002	AGS	C5-C6	2.74	1.48	1.41
3	H	2002	AGS	C5-C6	2.74	1.48	1.41
3	A	401	AGS	C5-C6	2.73	1.48	1.41
3	C	401	AGS	C5-C6	2.73	1.48	1.41
3	E	401	AGS	C5-C6	2.73	1.48	1.41
3	G	401	AGS	C5-C6	2.73	1.48	1.41
4	B	2001	GBM	C31-CL1	2.40	1.80	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2001	GBM	C31-CL1	2.40	1.80	1.74
4	F	2001	GBM	C31-CL1	2.40	1.80	1.74
4	H	2001	GBM	C31-CL1	2.40	1.80	1.74
3	A	401	AGS	C5-N7	-2.33	1.34	1.39
3	C	401	AGS	C5-N7	-2.33	1.34	1.39
3	E	401	AGS	C5-N7	-2.33	1.34	1.39
3	G	401	AGS	C5-N7	-2.33	1.34	1.39
3	B	2002	AGS	C8-N7	2.28	1.36	1.31
3	D	2002	AGS	C8-N7	2.28	1.36	1.31
3	F	2002	AGS	C8-N7	2.28	1.36	1.31
3	H	2002	AGS	C8-N7	2.28	1.36	1.31
3	B	2002	AGS	PB-O3A	2.23	1.61	1.59
3	D	2002	AGS	PB-O3A	2.23	1.61	1.59
3	F	2002	AGS	PB-O3A	2.23	1.61	1.59
3	H	2002	AGS	PB-O3A	2.23	1.61	1.59
3	B	2002	AGS	C5-N7	-2.23	1.35	1.39
3	D	2002	AGS	C5-N7	-2.23	1.35	1.39
3	F	2002	AGS	C5-N7	-2.23	1.35	1.39
3	H	2002	AGS	C5-N7	-2.23	1.35	1.39
3	A	401	AGS	C8-N7	2.22	1.35	1.31
3	C	401	AGS	C8-N7	2.22	1.35	1.31
3	E	401	AGS	C8-N7	2.22	1.35	1.31
3	G	401	AGS	C8-N7	2.22	1.35	1.31
4	B	2001	GBM	C17-N9	-2.21	1.34	1.39
4	D	2001	GBM	C17-N9	-2.21	1.34	1.39
4	F	2001	GBM	C17-N9	-2.21	1.34	1.39
4	H	2001	GBM	C17-N9	-2.21	1.34	1.39
3	A	401	AGS	PG-O2G	2.10	1.61	1.54
3	C	401	AGS	PG-O2G	2.10	1.61	1.54
3	E	401	AGS	PG-O2G	2.10	1.61	1.54
3	G	401	AGS	PG-O2G	2.10	1.61	1.54
3	B	2002	AGS	PG-O2G	2.10	1.61	1.54
3	D	2002	AGS	PG-O2G	2.10	1.61	1.54
3	F	2002	AGS	PG-O2G	2.10	1.61	1.54
3	H	2002	AGS	PG-O2G	2.10	1.61	1.54
3	B	2002	AGS	PA-O3A	2.06	1.61	1.59
3	D	2002	AGS	PA-O3A	2.06	1.61	1.59
3	F	2002	AGS	PA-O3A	2.06	1.61	1.59
3	H	2002	AGS	PA-O3A	2.06	1.61	1.59

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	GBM	O5-S2-O4	-9.79	107.64	119.52
4	D	2001	GBM	O5-S2-O4	-9.79	107.64	119.52
4	F	2001	GBM	O5-S2-O4	-9.79	107.64	119.52
4	H	2001	GBM	O5-S2-O4	-9.79	107.64	119.52
3	B	2002	AGS	C5-C4-N3	-5.92	118.57	126.72
3	D	2002	AGS	C5-C4-N3	-5.92	118.57	126.72
3	F	2002	AGS	C5-C4-N3	-5.92	118.57	126.72
3	H	2002	AGS	C5-C4-N3	-5.92	118.57	126.72
3	A	401	AGS	C5-C4-N3	-5.91	118.58	126.72
3	C	401	AGS	C5-C4-N3	-5.91	118.58	126.72
3	E	401	AGS	C5-C4-N3	-5.91	118.58	126.72
3	G	401	AGS	C5-C4-N3	-5.91	118.58	126.72
3	B	2002	AGS	N3-C4-N9	4.72	135.20	127.17
3	D	2002	AGS	N3-C4-N9	4.72	135.20	127.17
3	F	2002	AGS	N3-C4-N9	4.72	135.20	127.17
3	H	2002	AGS	N3-C4-N9	4.72	135.20	127.17
3	A	401	AGS	N3-C4-N9	4.71	135.17	127.17
3	C	401	AGS	N3-C4-N9	4.71	135.17	127.17
3	E	401	AGS	N3-C4-N9	4.71	135.17	127.17
3	G	401	AGS	N3-C4-N9	4.71	135.17	127.17
4	B	2001	GBM	O7-C28-C27	3.75	122.00	116.55
4	D	2001	GBM	O7-C28-C27	3.75	122.00	116.55
4	F	2001	GBM	O7-C28-C27	3.75	122.00	116.55
4	H	2001	GBM	O7-C28-C27	3.75	122.00	116.55
3	B	2002	AGS	C2-N3-C4	3.72	120.93	111.83
3	D	2002	AGS	C2-N3-C4	3.72	120.93	111.83
3	F	2002	AGS	C2-N3-C4	3.72	120.93	111.83
3	H	2002	AGS	C2-N3-C4	3.72	120.93	111.83
3	A	401	AGS	C2-N3-C4	3.67	120.79	111.83
3	C	401	AGS	C2-N3-C4	3.67	120.79	111.83
3	E	401	AGS	C2-N3-C4	3.67	120.79	111.83
3	G	401	AGS	C2-N3-C4	3.67	120.79	111.83
3	B	2002	AGS	C4-C5-N7	-3.40	106.69	110.58
3	D	2002	AGS	C4-C5-N7	-3.40	106.69	110.58
3	F	2002	AGS	C4-C5-N7	-3.40	106.69	110.58
3	H	2002	AGS	C4-C5-N7	-3.40	106.69	110.58
3	A	401	AGS	C4-C5-N7	-3.40	106.70	110.58
3	C	401	AGS	C4-C5-N7	-3.40	106.70	110.58
3	E	401	AGS	C4-C5-N7	-3.40	106.70	110.58
3	G	401	AGS	C4-C5-N7	-3.40	106.70	110.58
3	A	401	AGS	PB-O3B-PG	-3.33	120.98	133.17
3	C	401	AGS	PB-O3B-PG	-3.33	120.98	133.17
3	E	401	AGS	PB-O3B-PG	-3.33	120.98	133.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	401	AGS	PB-O3B-PG	-3.33	120.98	133.17
3	B	2002	AGS	PB-O3B-PG	-3.29	121.14	133.17
3	D	2002	AGS	PB-O3B-PG	-3.29	121.14	133.17
3	F	2002	AGS	PB-O3B-PG	-3.29	121.14	133.17
3	H	2002	AGS	PB-O3B-PG	-3.29	121.14	133.17
3	B	2002	AGS	N3-C2-N1	-3.22	123.71	128.58
3	D	2002	AGS	N3-C2-N1	-3.22	123.71	128.58
3	F	2002	AGS	N3-C2-N1	-3.22	123.71	128.58
3	H	2002	AGS	N3-C2-N1	-3.22	123.71	128.58
3	A	401	AGS	N3-C2-N1	-3.14	123.83	128.58
3	C	401	AGS	N3-C2-N1	-3.14	123.83	128.58
3	E	401	AGS	N3-C2-N1	-3.14	123.83	128.58
3	G	401	AGS	N3-C2-N1	-3.14	123.83	128.58
4	B	2001	GBM	C18-S2-N9	3.03	110.89	106.06
4	D	2001	GBM	C18-S2-N9	3.03	110.89	106.06
4	F	2001	GBM	C18-S2-N9	3.03	110.89	106.06
4	H	2001	GBM	C18-S2-N9	3.03	110.89	106.06
4	B	2001	GBM	O7-C28-C30	-2.90	119.41	124.30
4	D	2001	GBM	O7-C28-C30	-2.90	119.41	124.30
4	F	2001	GBM	O7-C28-C30	-2.90	119.41	124.30
4	H	2001	GBM	O7-C28-C30	-2.90	119.41	124.30
3	B	2002	AGS	C4-N9-C8	2.62	108.48	105.74
3	D	2002	AGS	C4-N9-C8	2.62	108.48	105.74
3	F	2002	AGS	C4-N9-C8	2.62	108.48	105.74
3	H	2002	AGS	C4-N9-C8	2.62	108.48	105.74
3	B	2002	AGS	C3'-C2'-C1'	2.49	106.17	101.46
3	D	2002	AGS	C3'-C2'-C1'	2.49	106.17	101.46
3	F	2002	AGS	C3'-C2'-C1'	2.49	106.17	101.46
3	H	2002	AGS	C3'-C2'-C1'	2.49	106.17	101.46
3	B	2002	AGS	C5-N7-C8	2.48	107.35	103.45
3	D	2002	AGS	C5-N7-C8	2.48	107.35	103.45
3	F	2002	AGS	C5-N7-C8	2.48	107.35	103.45
3	H	2002	AGS	C5-N7-C8	2.48	107.35	103.45
3	A	401	AGS	C4-N9-C8	2.45	108.31	105.74
3	C	401	AGS	C4-N9-C8	2.45	108.31	105.74
3	E	401	AGS	C4-N9-C8	2.45	108.31	105.74
3	G	401	AGS	C4-N9-C8	2.45	108.31	105.74
3	A	401	AGS	C5-N7-C8	2.44	107.28	103.45
3	C	401	AGS	C5-N7-C8	2.44	107.28	103.45
3	E	401	AGS	C5-N7-C8	2.44	107.28	103.45
3	G	401	AGS	C5-N7-C8	2.44	107.28	103.45
3	A	401	AGS	C3'-C2'-C1'	2.44	106.08	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	AGS	C3'-C2'-C1'	2.44	106.08	101.46
3	E	401	AGS	C3'-C2'-C1'	2.44	106.08	101.46
3	G	401	AGS	C3'-C2'-C1'	2.44	106.08	101.46
4	B	2001	GBM	C25-C20-C19	-2.31	107.62	112.83
4	D	2001	GBM	C25-C20-C19	-2.31	107.62	112.83
4	F	2001	GBM	C25-C20-C19	-2.31	107.62	112.83
4	H	2001	GBM	C25-C20-C19	-2.31	107.62	112.83
4	B	2001	GBM	C28-C27-C26	-2.13	122.40	126.24
4	D	2001	GBM	C28-C27-C26	-2.13	122.40	126.24
4	F	2001	GBM	C28-C27-C26	-2.13	122.40	126.24
4	H	2001	GBM	C28-C27-C26	-2.13	122.40	126.24
4	B	2001	GBM	C33-O7-C28	2.12	120.62	117.51
4	D	2001	GBM	C33-O7-C28	2.12	120.62	117.51
4	F	2001	GBM	C33-O7-C28	2.12	120.62	117.51
4	H	2001	GBM	C33-O7-C28	2.12	120.62	117.51

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2002	AGS	PB-O3B-PG-O2G
3	B	2002	AGS	PB-O3B-PG-O3G
3	D	2002	AGS	PB-O3B-PG-O2G
3	D	2002	AGS	PB-O3B-PG-O3G
3	F	2002	AGS	PB-O3B-PG-O2G
3	F	2002	AGS	PB-O3B-PG-O3G
3	H	2002	AGS	PB-O3B-PG-O2G
3	H	2002	AGS	PB-O3B-PG-O3G
4	B	2001	GBM	C27-C26-N10-C25
4	D	2001	GBM	C27-C26-N10-C25
4	F	2001	GBM	C27-C26-N10-C25
4	H	2001	GBM	C27-C26-N10-C25
4	B	2001	GBM	O6-C26-N10-C25
4	D	2001	GBM	O6-C26-N10-C25
4	F	2001	GBM	O6-C26-N10-C25
4	H	2001	GBM	O6-C26-N10-C25
4	B	2001	GBM	O3-C17-N8-C11
4	D	2001	GBM	O3-C17-N8-C11
4	F	2001	GBM	O3-C17-N8-C11
4	H	2001	GBM	O3-C17-N8-C11
4	B	2001	GBM	C30-C28-O7-C33
4	D	2001	GBM	C30-C28-O7-C33

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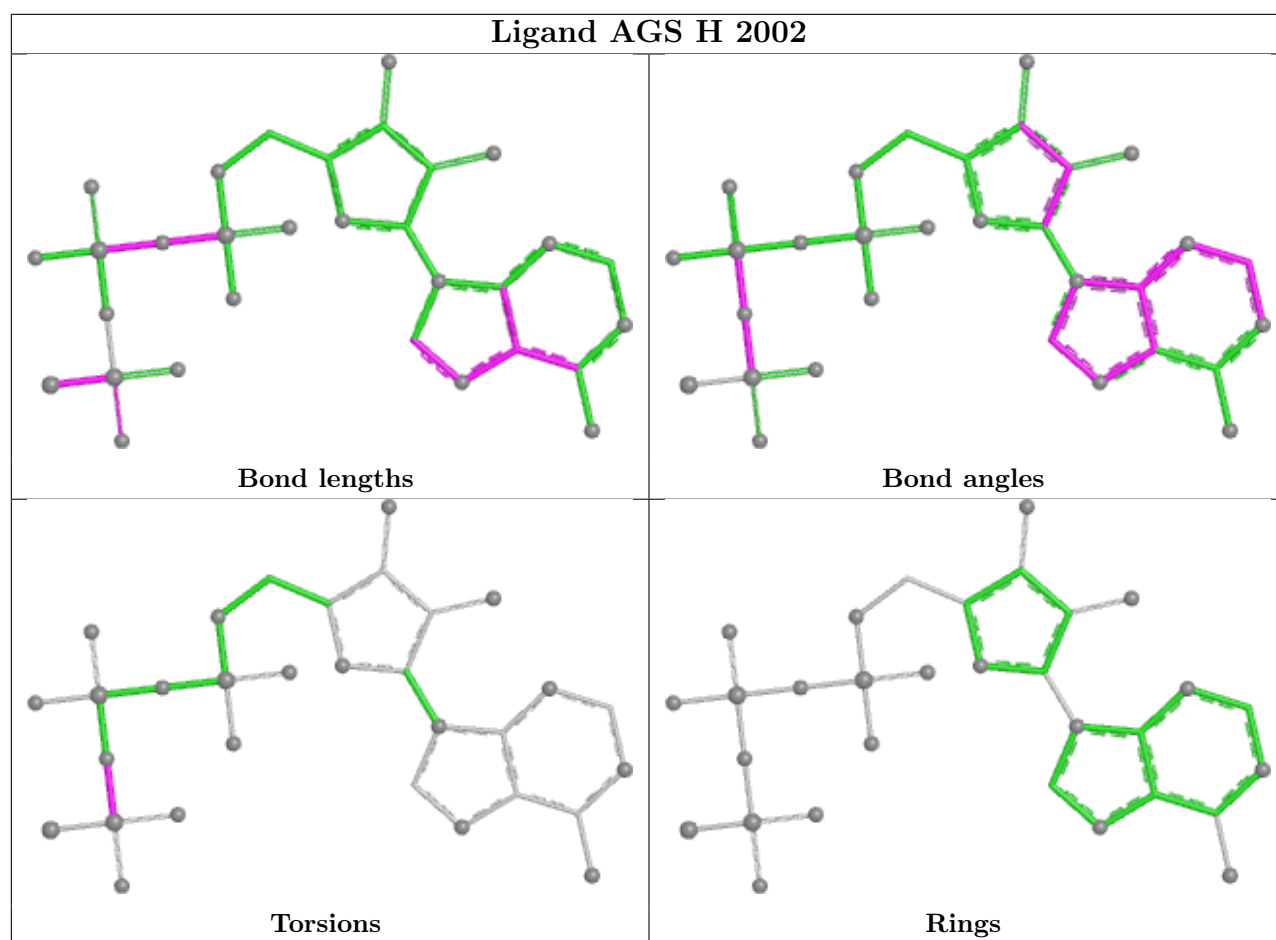
Mol	Chain	Res	Type	Atoms
4	F	2001	GBM	C30-C28-O7-C33
4	H	2001	GBM	C30-C28-O7-C33
4	B	2001	GBM	C27-C28-O7-C33
4	D	2001	GBM	C27-C28-O7-C33
4	F	2001	GBM	C27-C28-O7-C33
4	H	2001	GBM	C27-C28-O7-C33
3	A	401	AGS	O4'-C4'-C5'-O5'
3	C	401	AGS	O4'-C4'-C5'-O5'
3	E	401	AGS	O4'-C4'-C5'-O5'
3	G	401	AGS	O4'-C4'-C5'-O5'
3	A	401	AGS	PB-O3A-PA-O1A
3	C	401	AGS	PB-O3A-PA-O1A
3	E	401	AGS	PB-O3A-PA-O1A
3	G	401	AGS	PB-O3A-PA-O1A
4	B	2001	GBM	N9-C17-N8-C11
4	D	2001	GBM	N9-C17-N8-C11
4	F	2001	GBM	N9-C17-N8-C11
4	H	2001	GBM	N9-C17-N8-C11
4	B	2001	GBM	C24-C19-C20-C25
4	D	2001	GBM	C24-C19-C20-C25
4	F	2001	GBM	C24-C19-C20-C25
4	H	2001	GBM	C24-C19-C20-C25
4	B	2001	GBM	C23-C19-C20-C25
4	D	2001	GBM	C23-C19-C20-C25
4	F	2001	GBM	C23-C19-C20-C25
4	H	2001	GBM	C23-C19-C20-C25
3	A	401	AGS	PB-O3A-PA-O2A
3	C	401	AGS	PB-O3A-PA-O2A
3	E	401	AGS	PB-O3A-PA-O2A
3	G	401	AGS	PB-O3A-PA-O2A
3	A	401	AGS	C2'-C1'-N9-C8
3	C	401	AGS	C2'-C1'-N9-C8
3	E	401	AGS	C2'-C1'-N9-C8
3	G	401	AGS	C2'-C1'-N9-C8
3	A	401	AGS	C3'-C4'-C5'-O5'
3	C	401	AGS	C3'-C4'-C5'-O5'
3	E	401	AGS	C3'-C4'-C5'-O5'
3	G	401	AGS	C3'-C4'-C5'-O5'

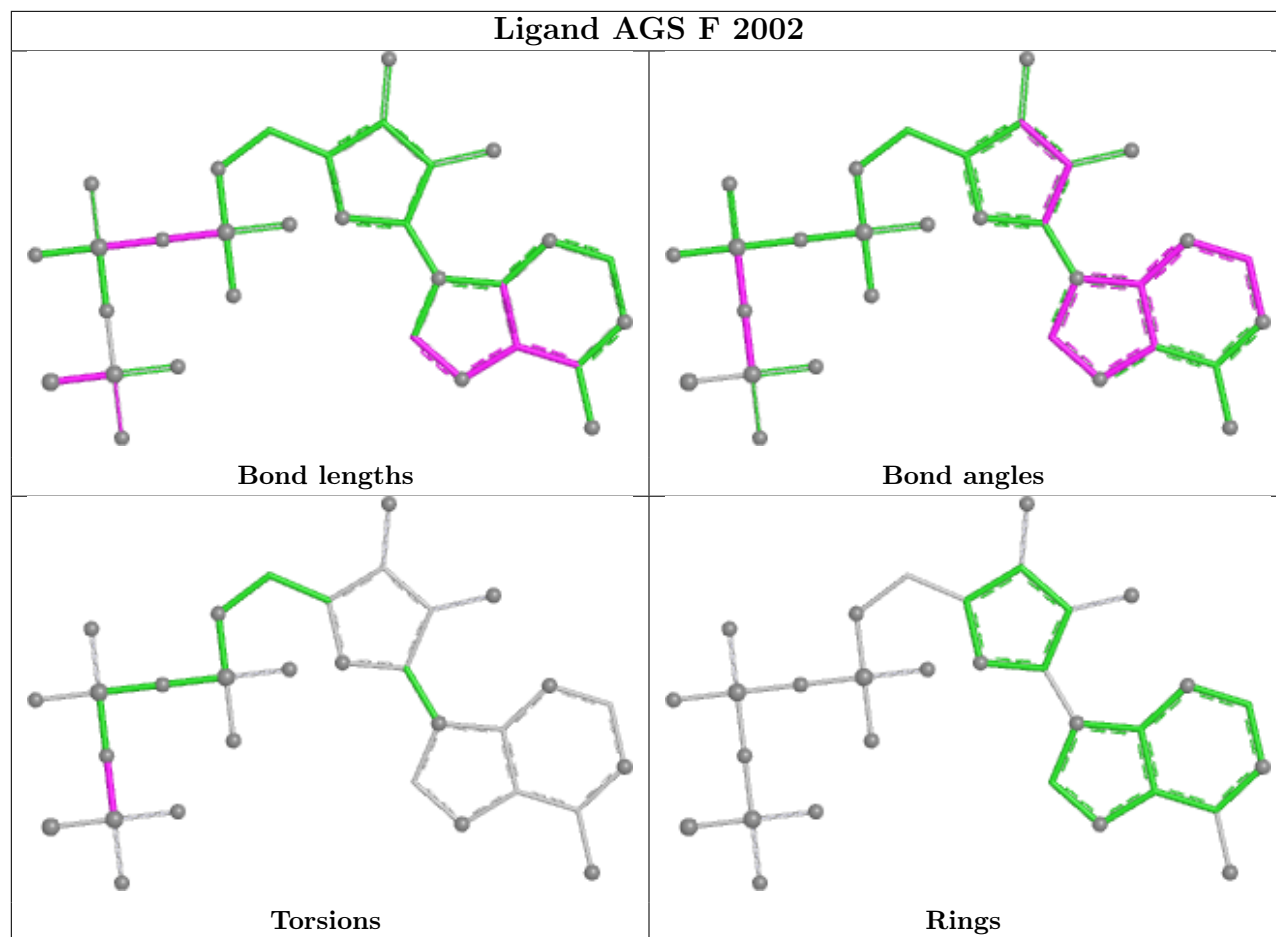
There are no ring outliers.

12 monomers are involved in 30 short contacts:

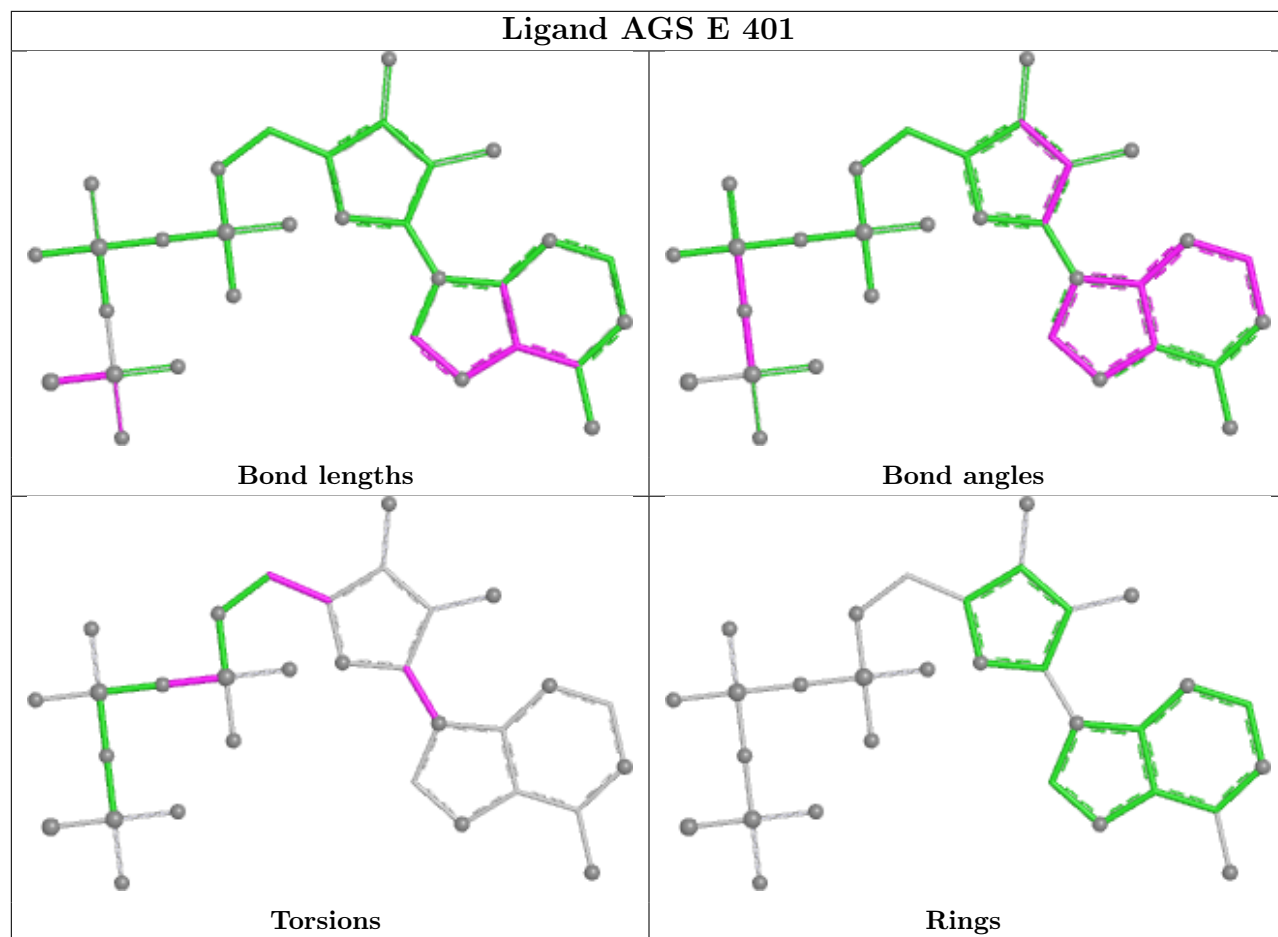
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	2002	AGS	2	0
3	F	2002	AGS	2	0
3	E	401	AGS	2	0
3	A	401	AGS	2	0
3	B	2002	AGS	2	0
4	D	2001	GBM	4	0
4	H	2001	GBM	3	0
3	C	401	AGS	2	0
4	F	2001	GBM	3	0
3	D	2002	AGS	2	0
4	B	2001	GBM	4	0
3	G	401	AGS	2	0

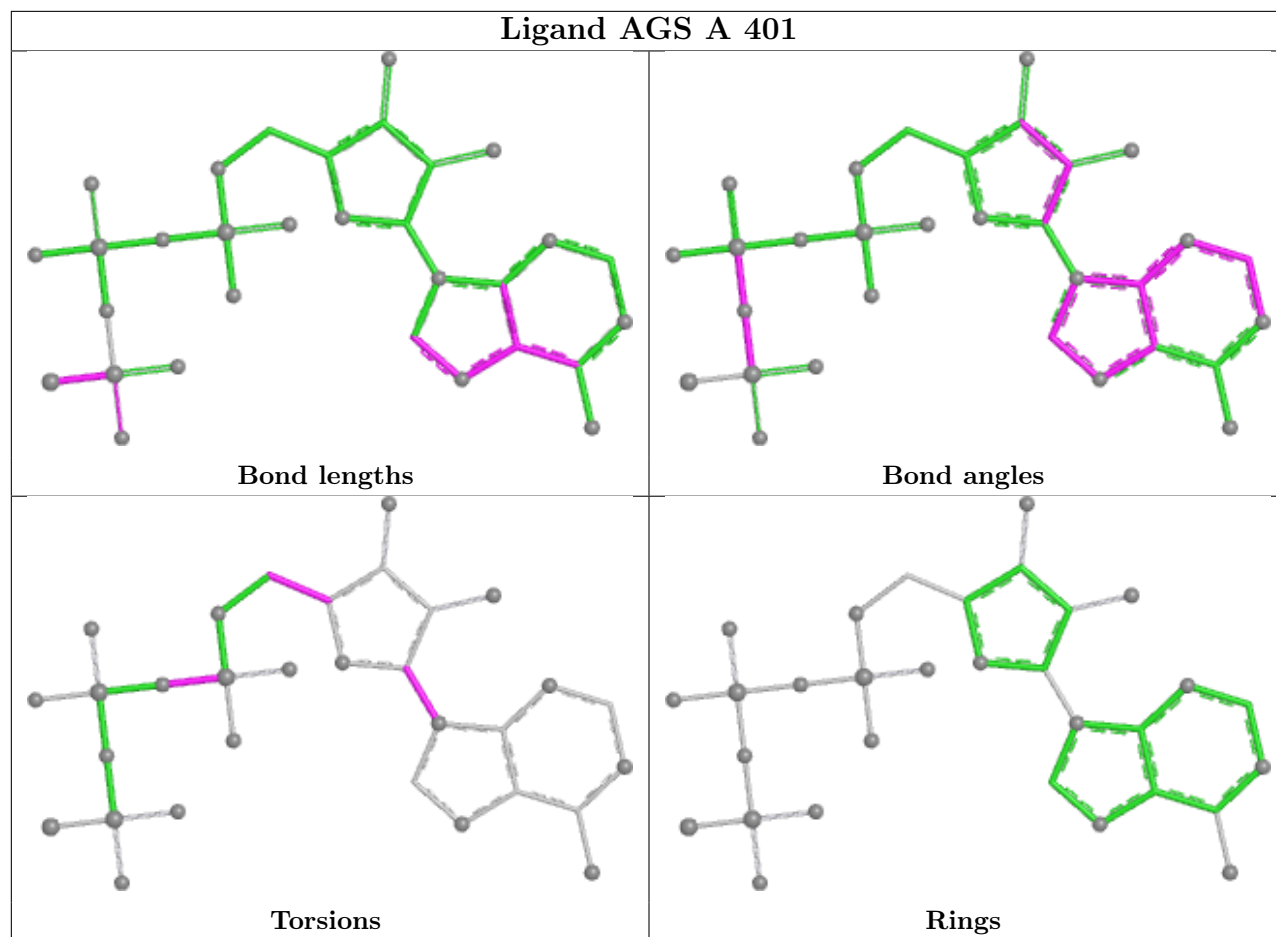
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

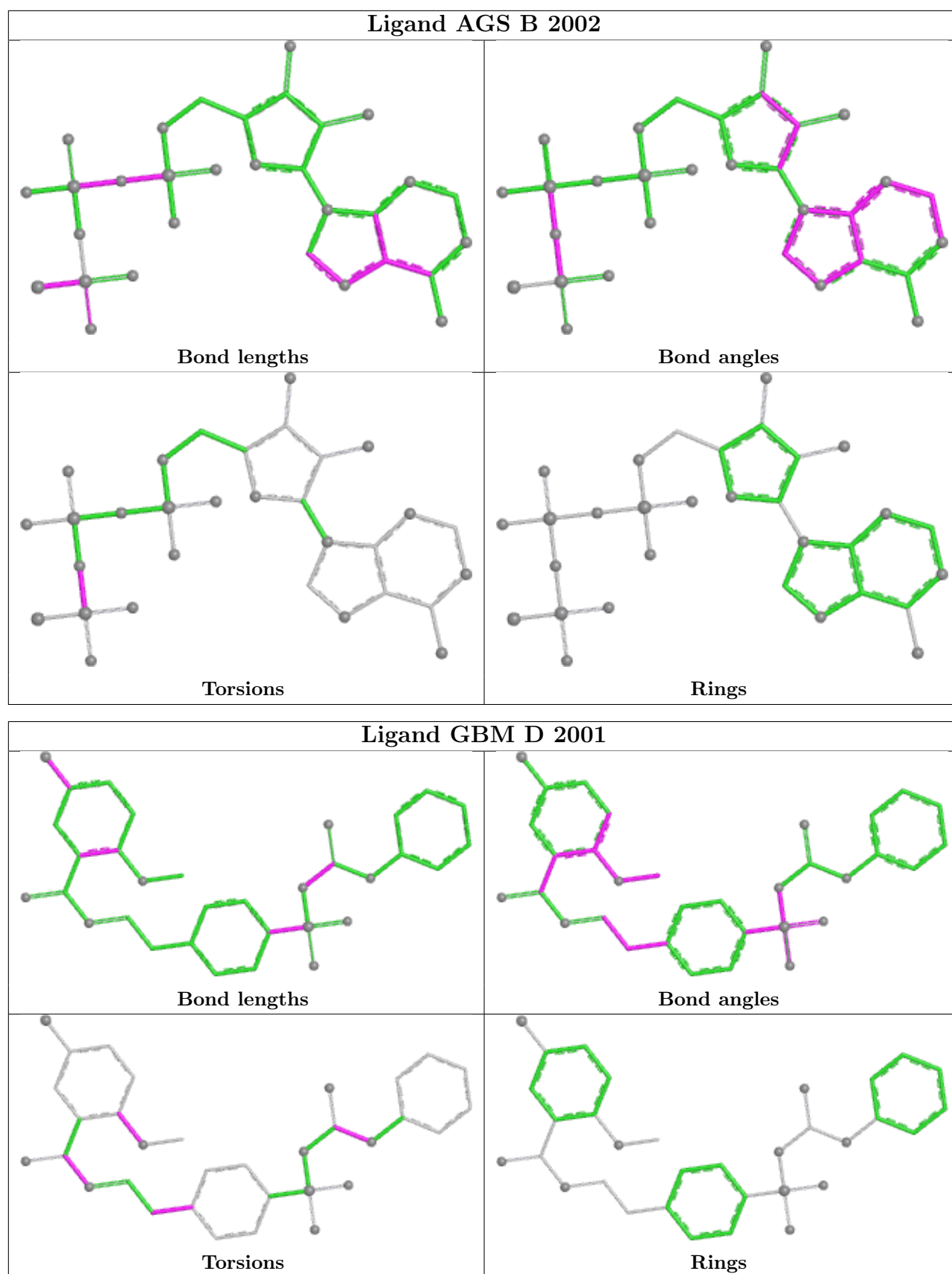




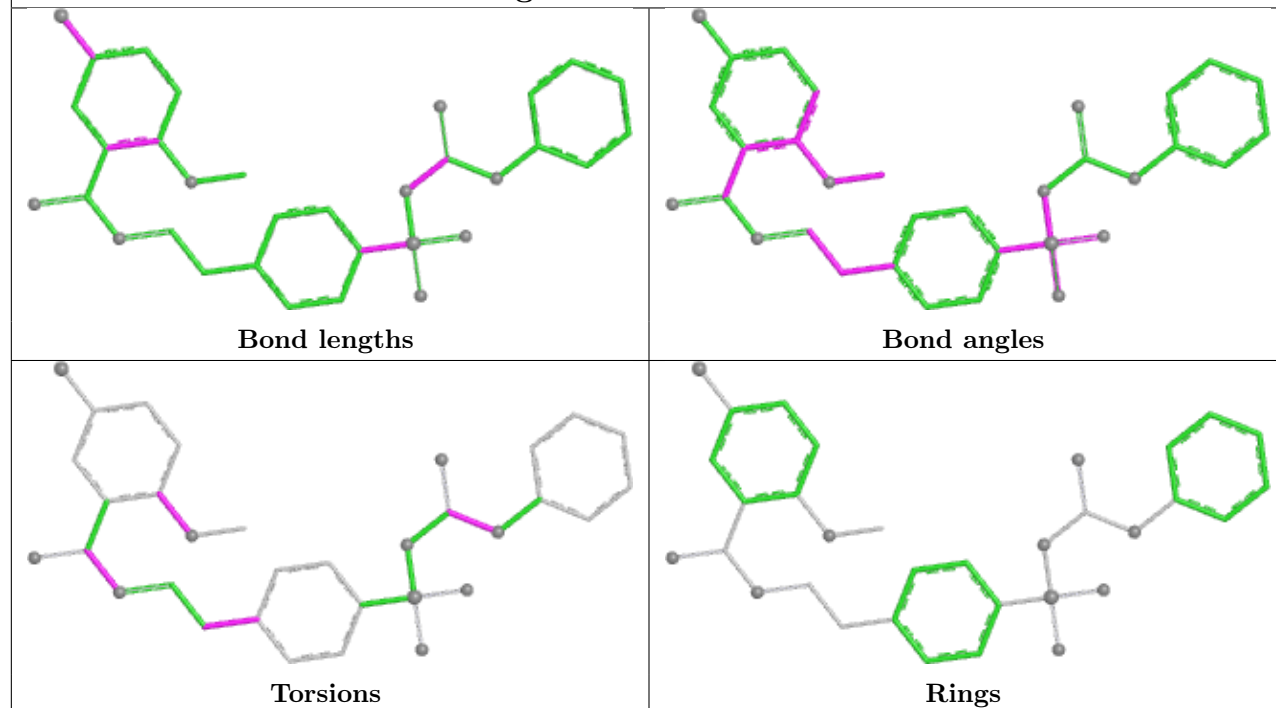
Ligand AGS E 401



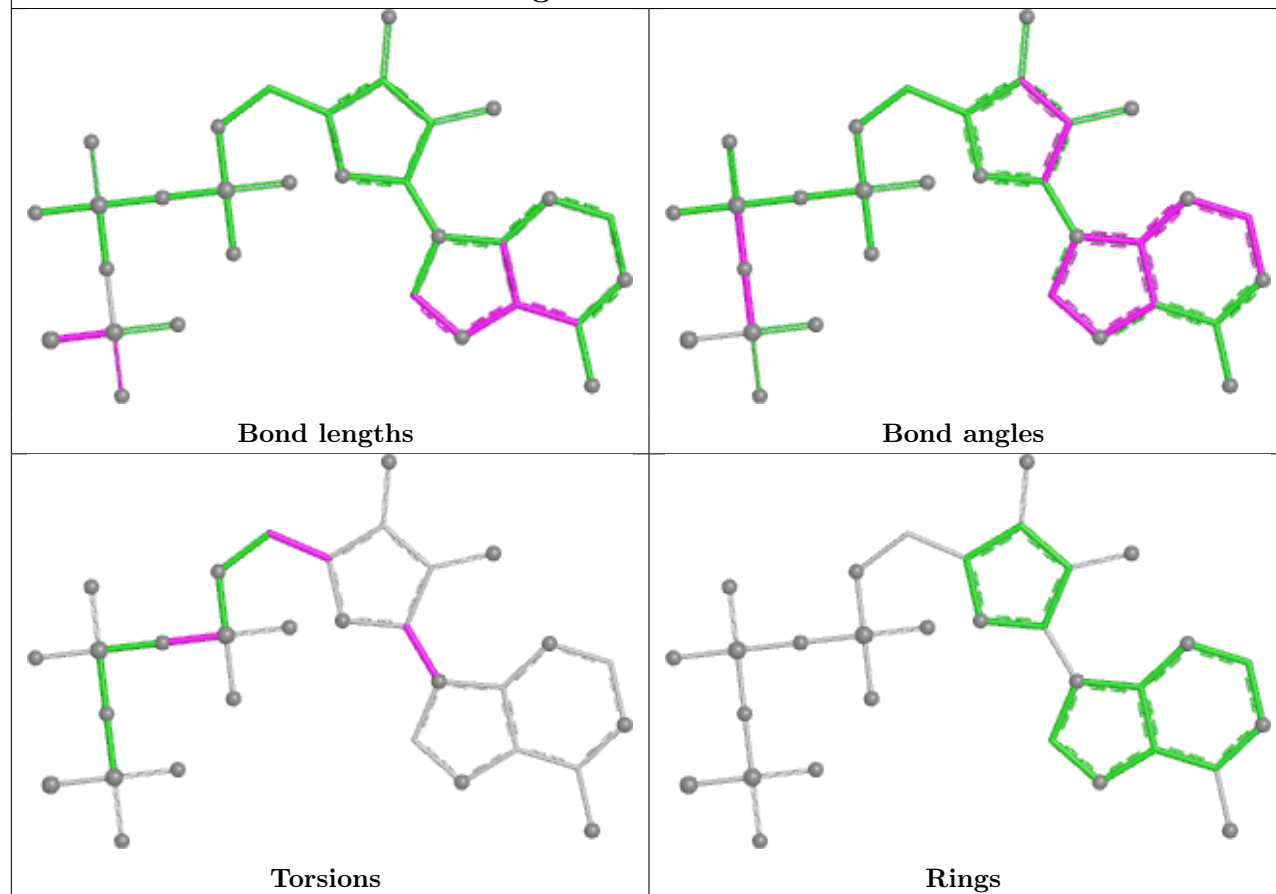




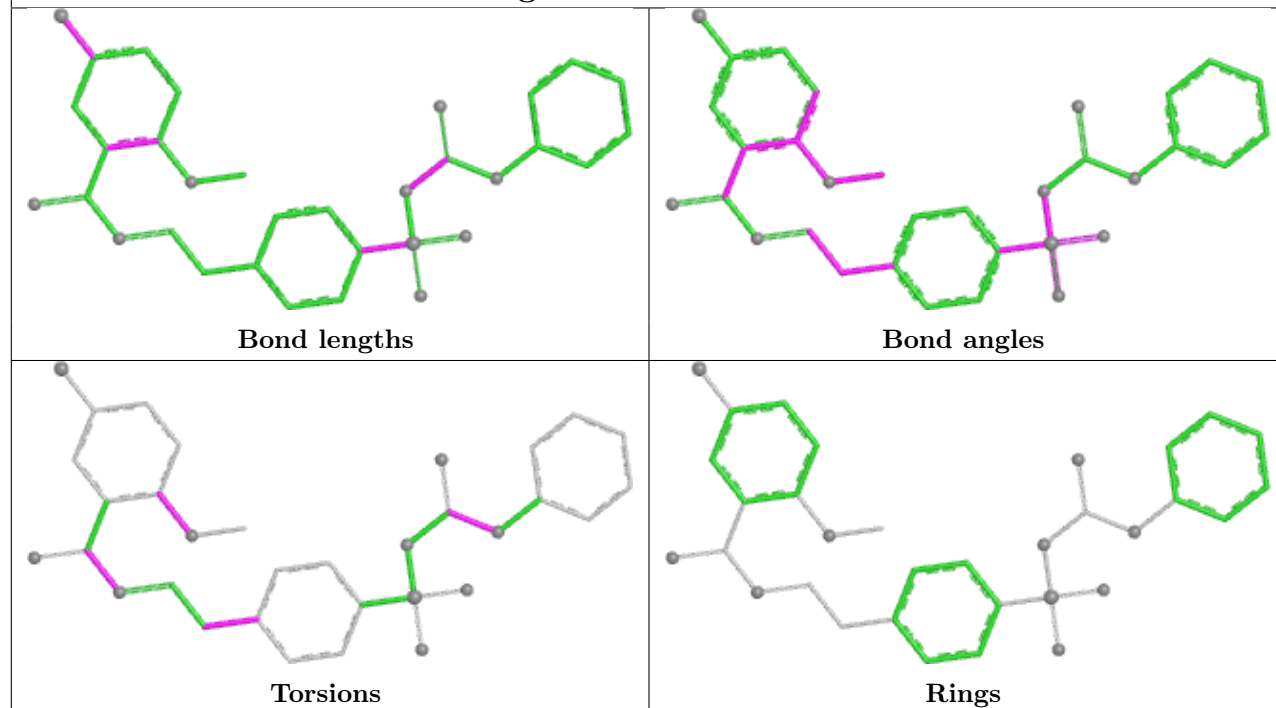
Ligand GBM H 2001



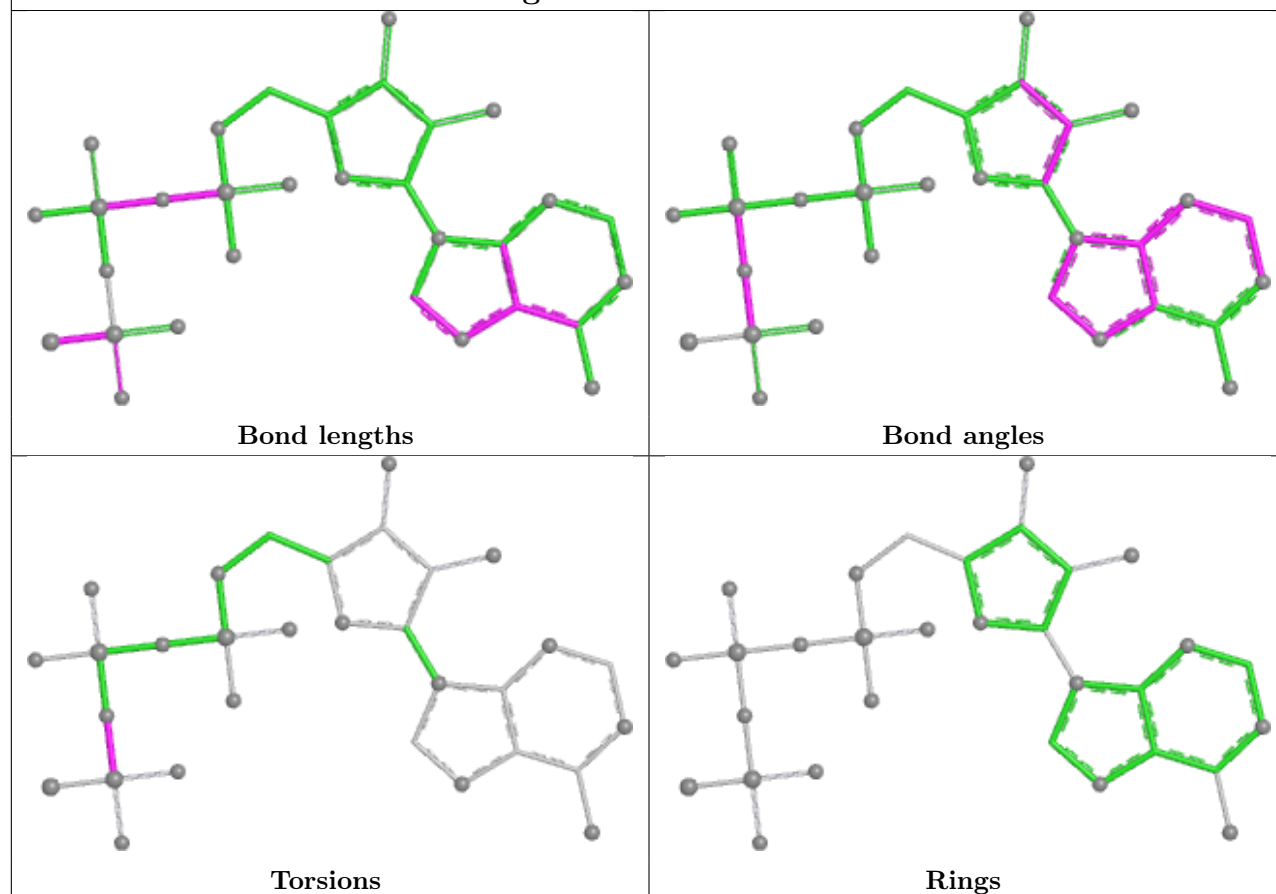
Ligand AGS C 401



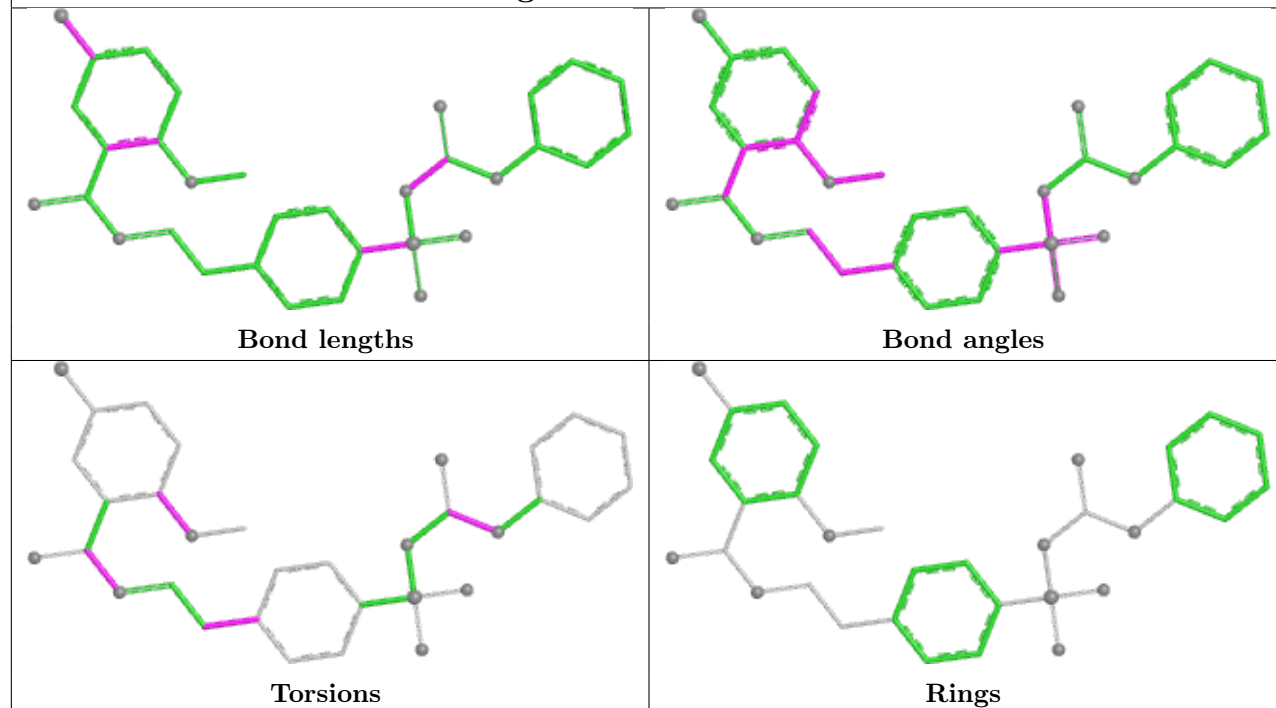
Ligand GBM F 2001



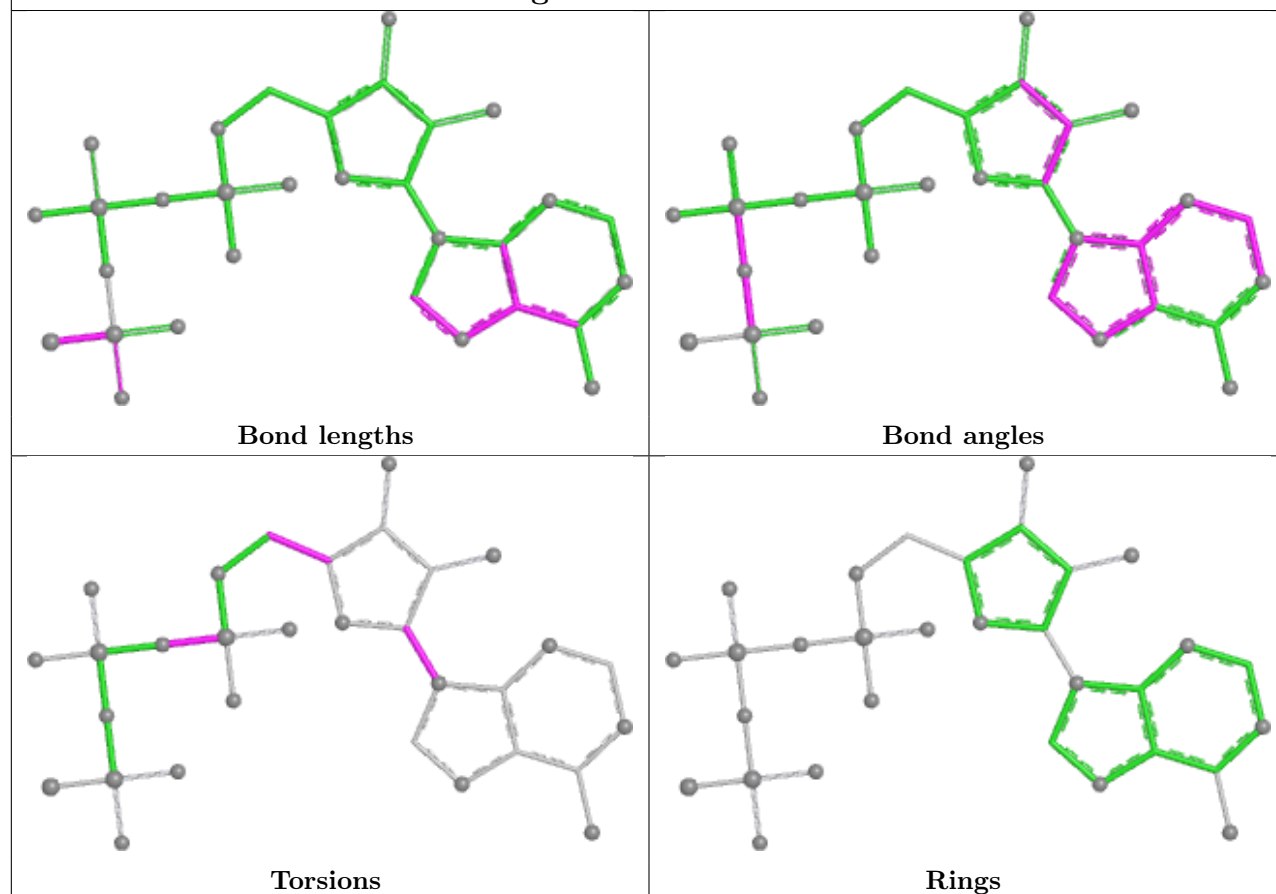
Ligand AGS D 2002



Ligand GBM B 2001



Ligand AGS G 401



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

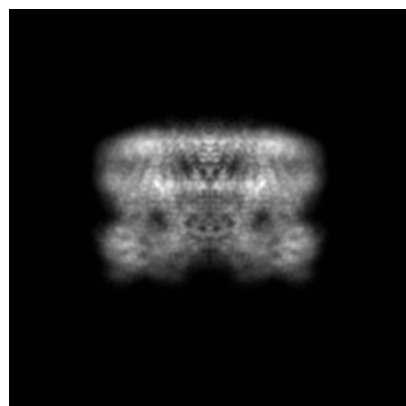
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6833. These allow visual inspection of the internal detail of the map and identification of artifacts.

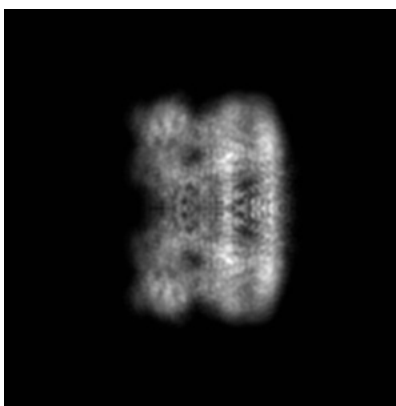
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

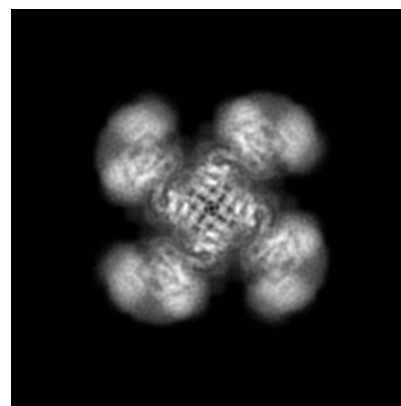
6.1.1 Primary map



X

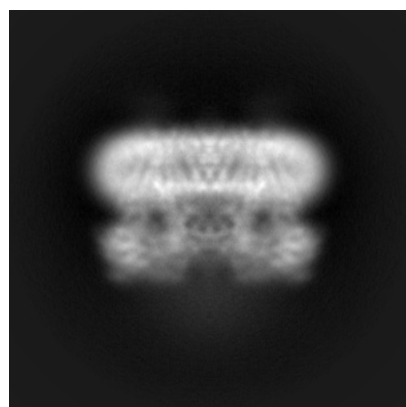


Y

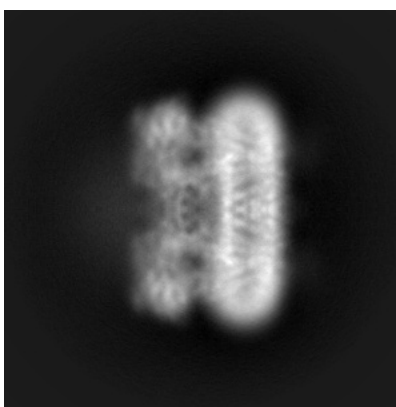


Z

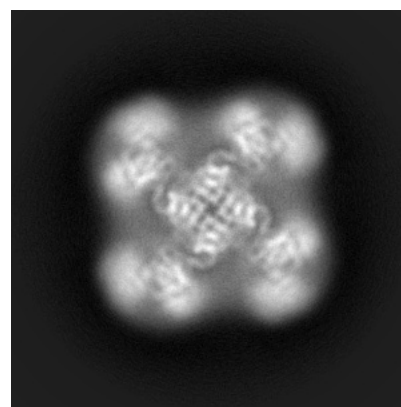
6.1.2 Raw map



X



Y



Z

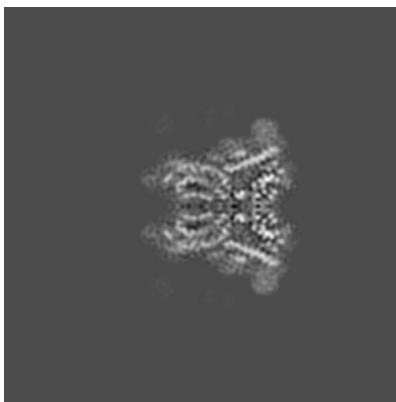
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

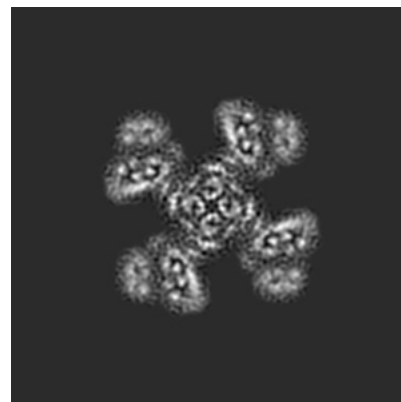
6.2.1 Primary map



X Index: 156

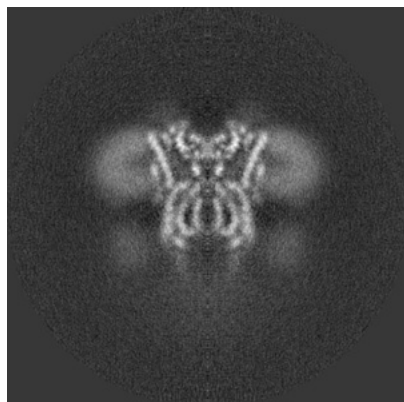


Y Index: 156

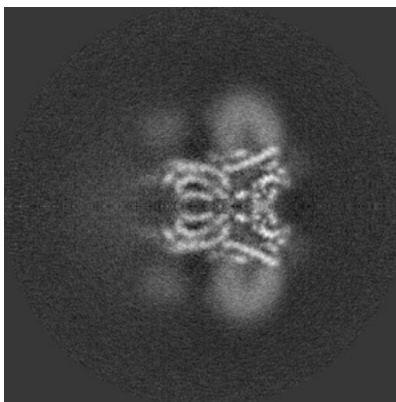


Z Index: 156

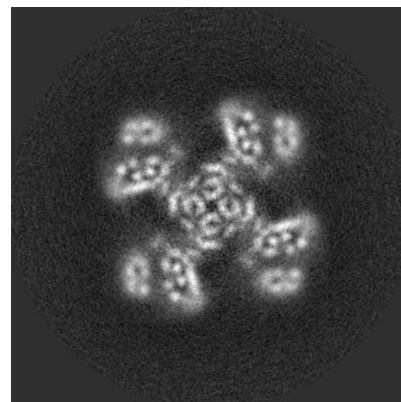
6.2.2 Raw map



X Index: 156



Y Index: 156

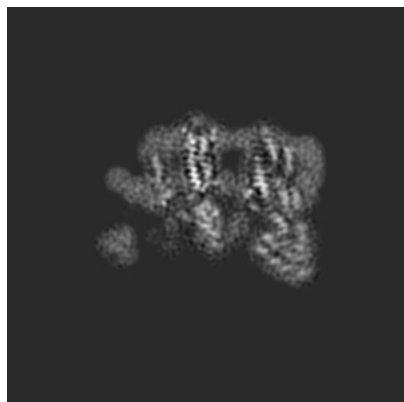


Z Index: 156

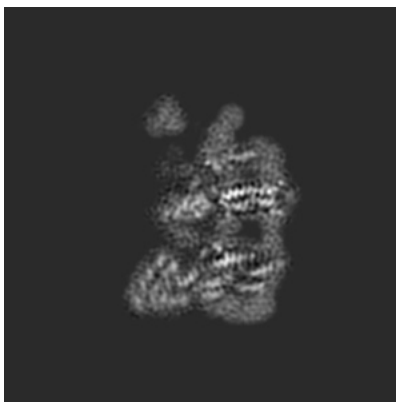
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

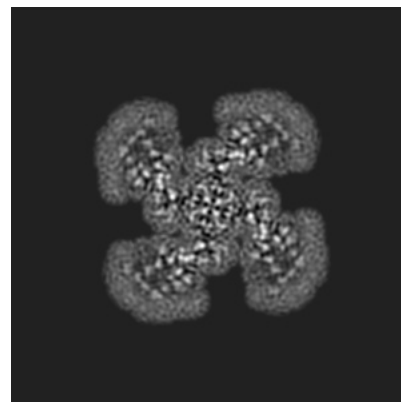
6.3.1 Primary map



X Index: 187

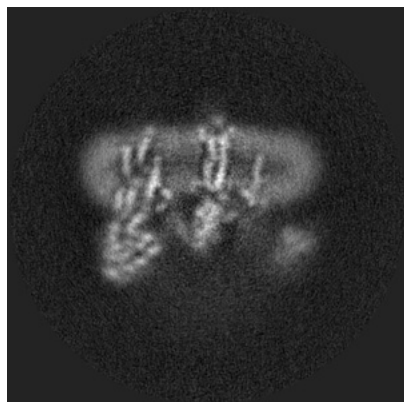


Y Index: 187

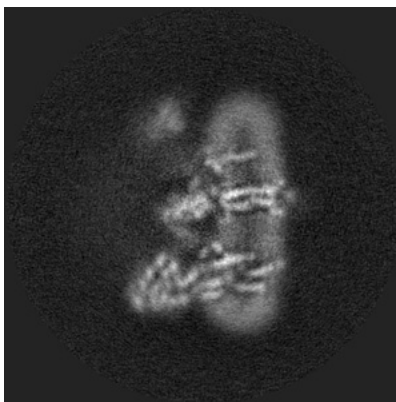


Z Index: 175

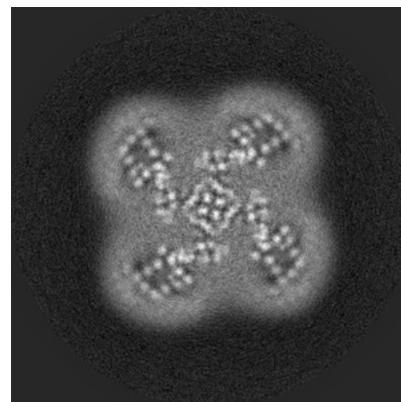
6.3.2 Raw map



X Index: 125



Y Index: 187

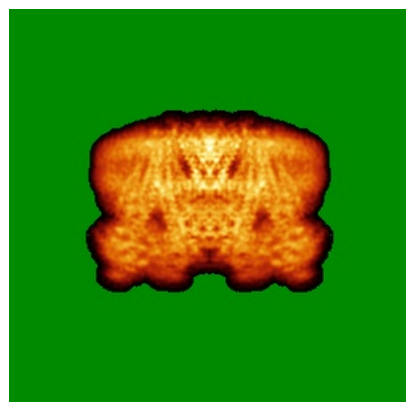


Z Index: 174

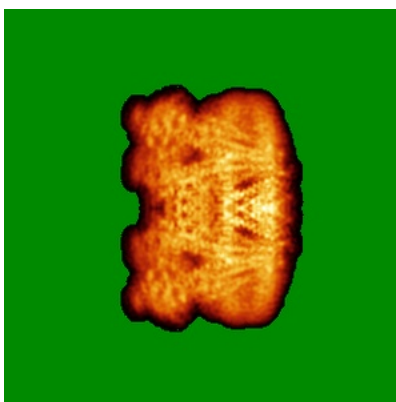
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

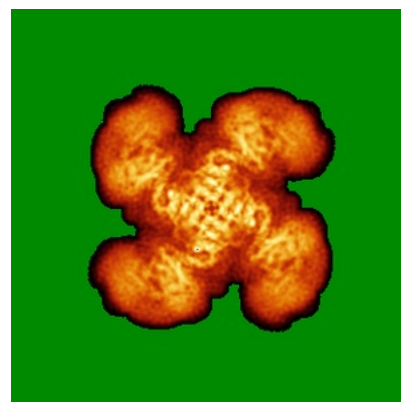
6.4.1 Primary map



X



Y

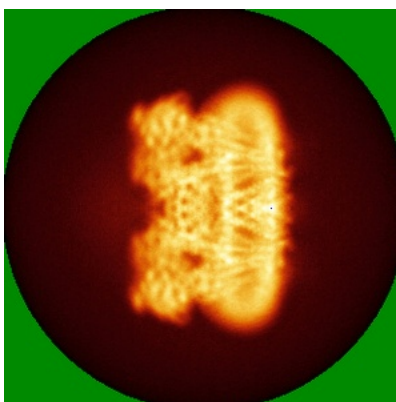


Z

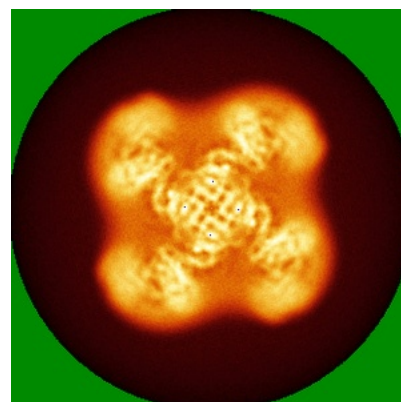
6.4.2 Raw map



X



Y

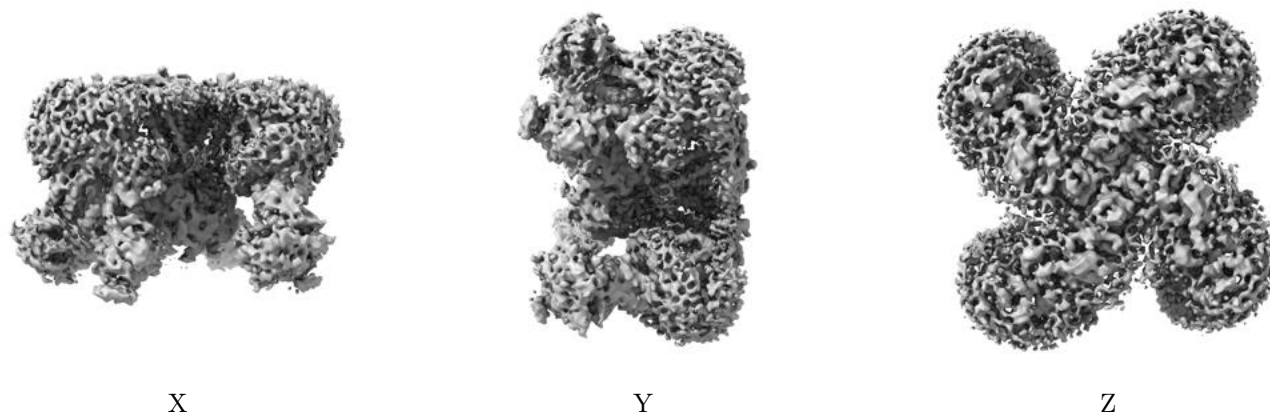


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

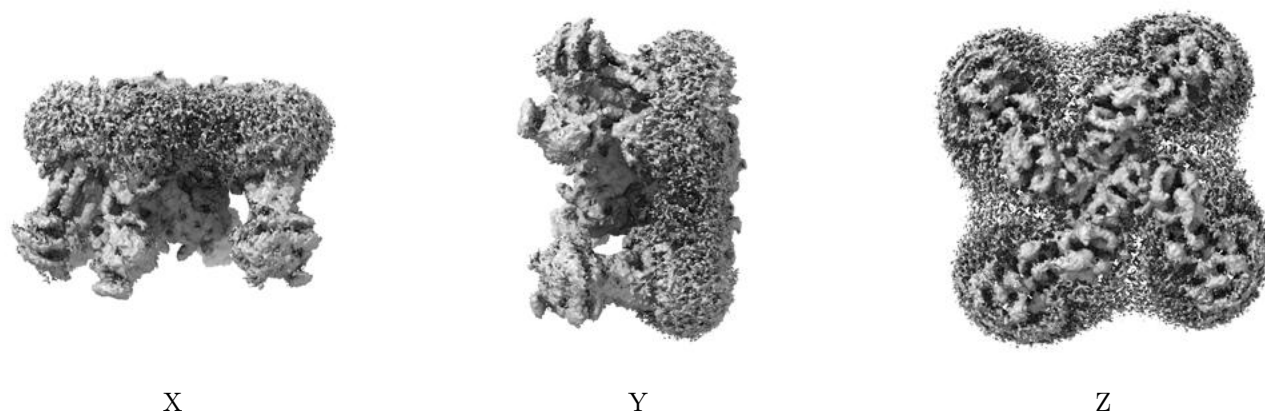
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

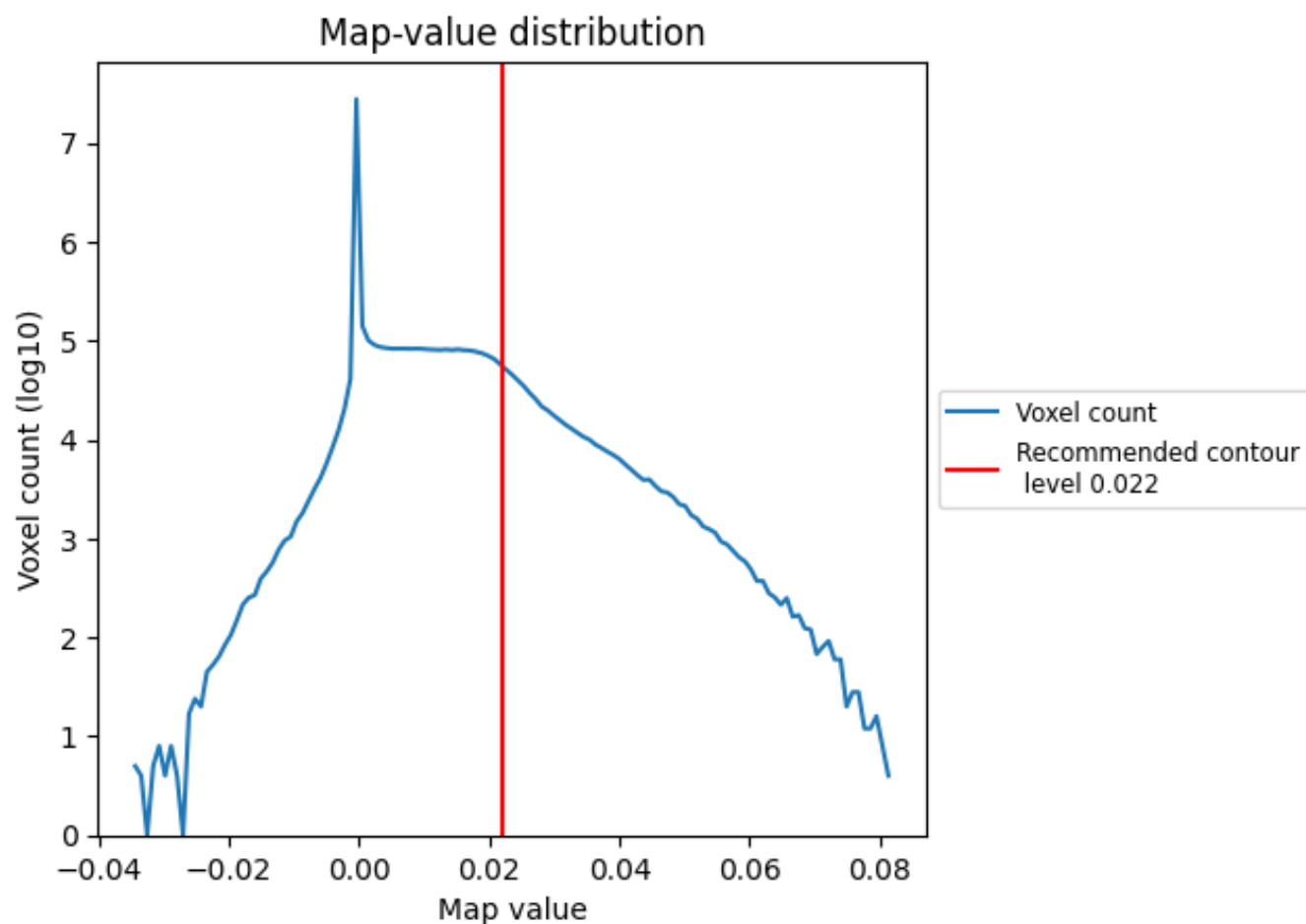
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

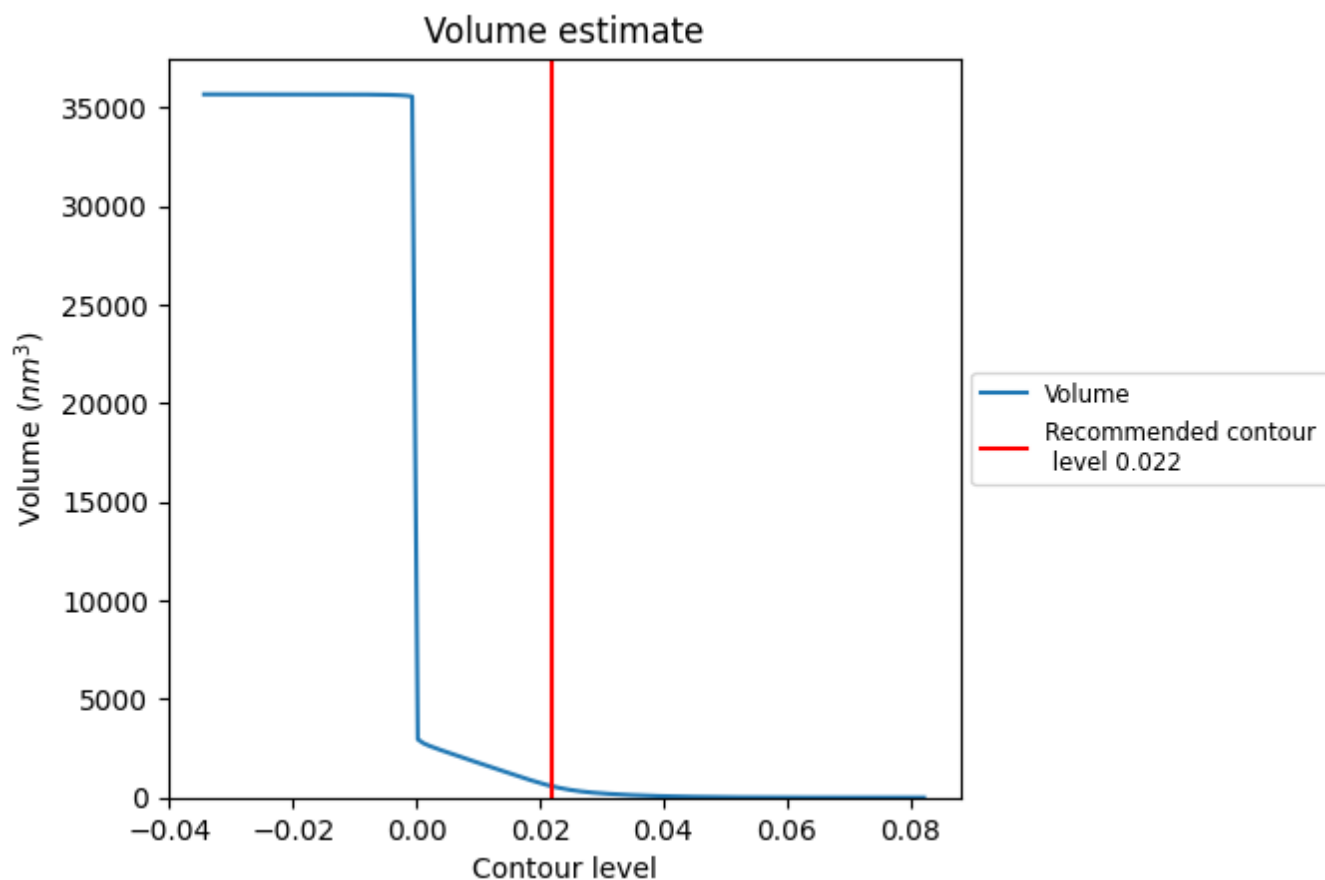
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

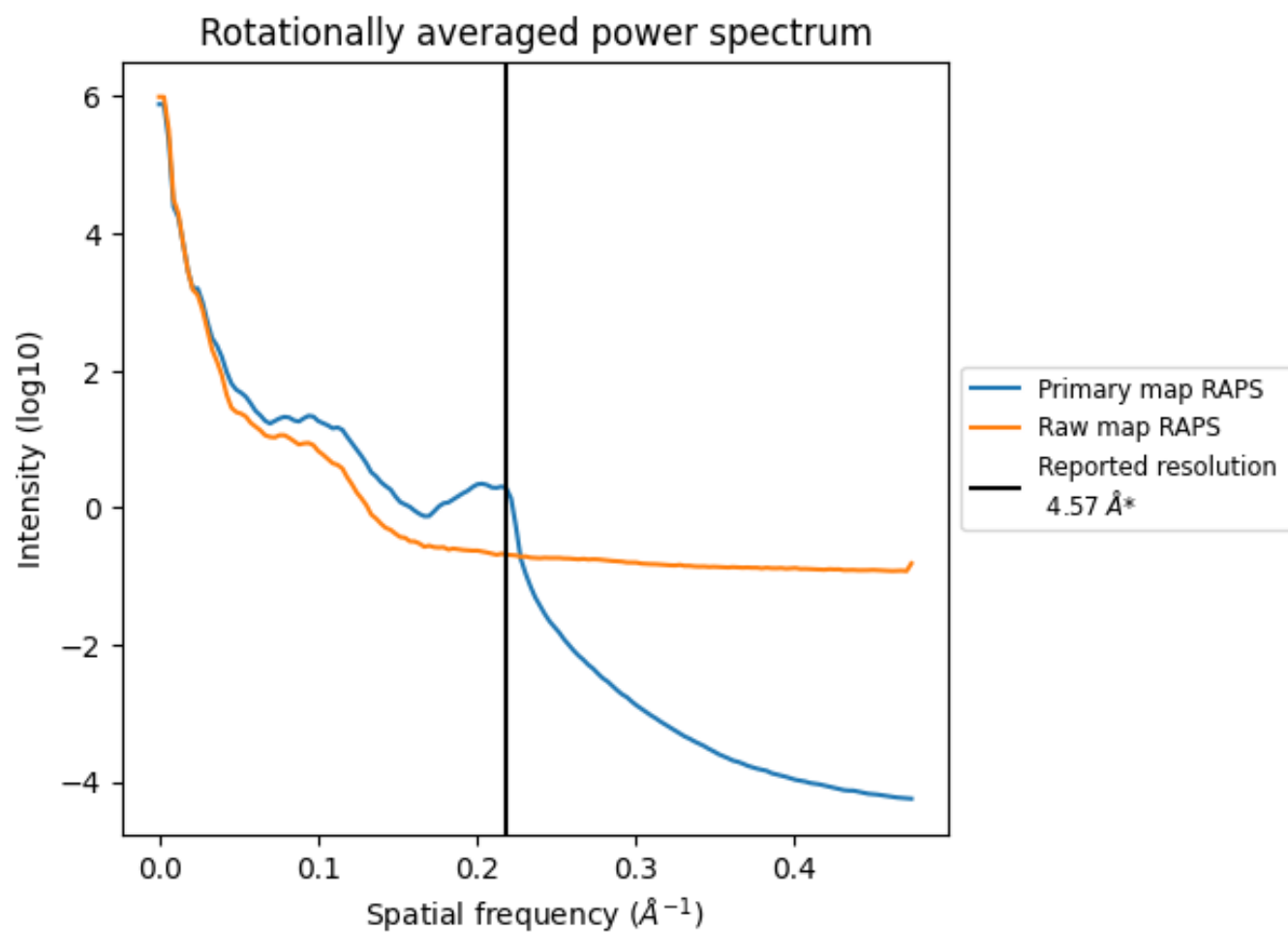
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 573 nm³; this corresponds to an approximate mass of 517 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

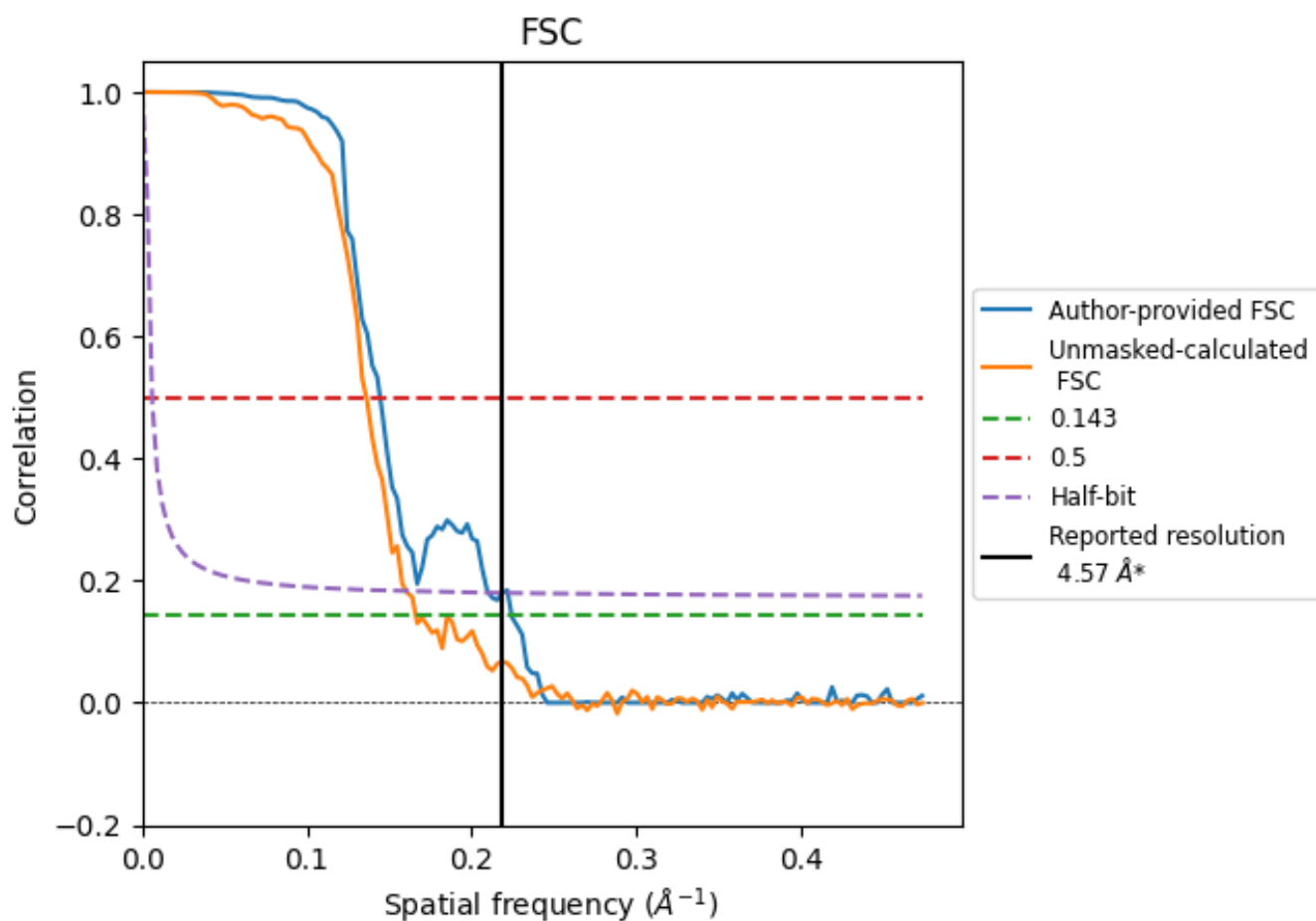


*Reported resolution corresponds to spatial frequency of 0.219 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.219 Å⁻¹

8.2 Resolution estimates [i](#)

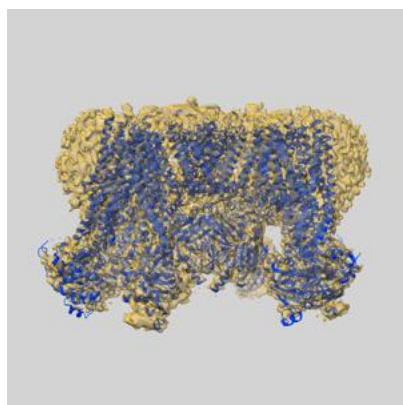
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.57	-	-
Author-provided FSC curve	4.45	6.92	4.75
Unmasked-calculated*	6.02	7.35	6.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.02 differs from the reported value 4.57 by more than 10 %

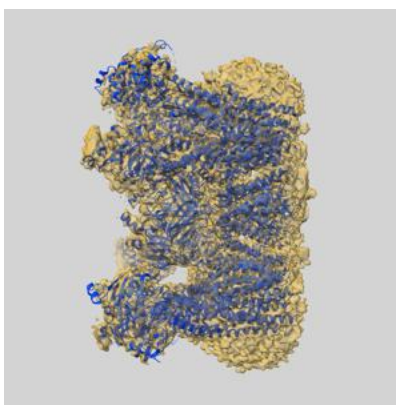
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6833 and PDB model 5YKG. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

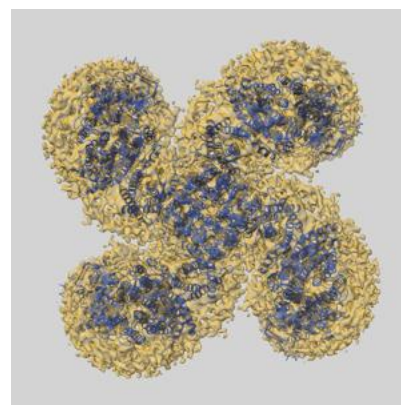
9.1 Map-model overlay [i](#)



X



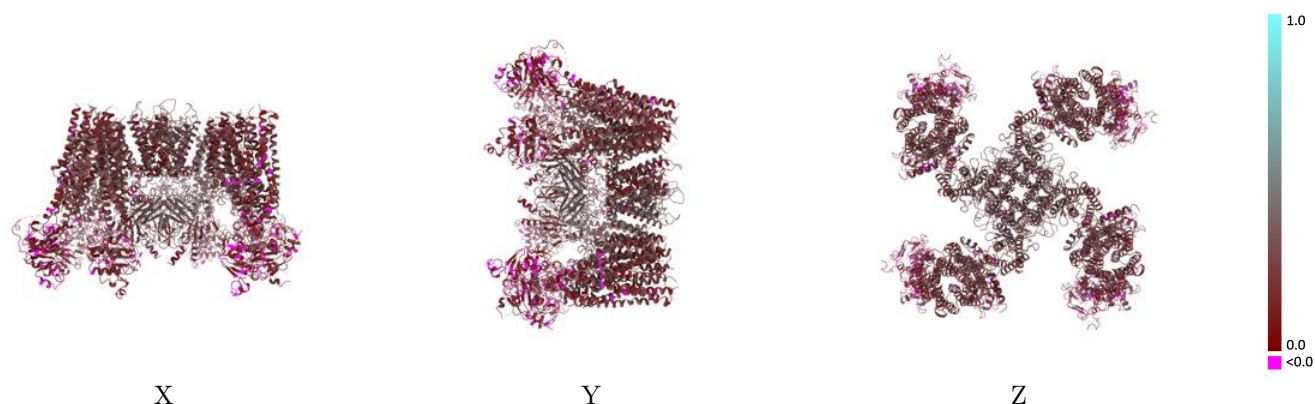
Y



Z

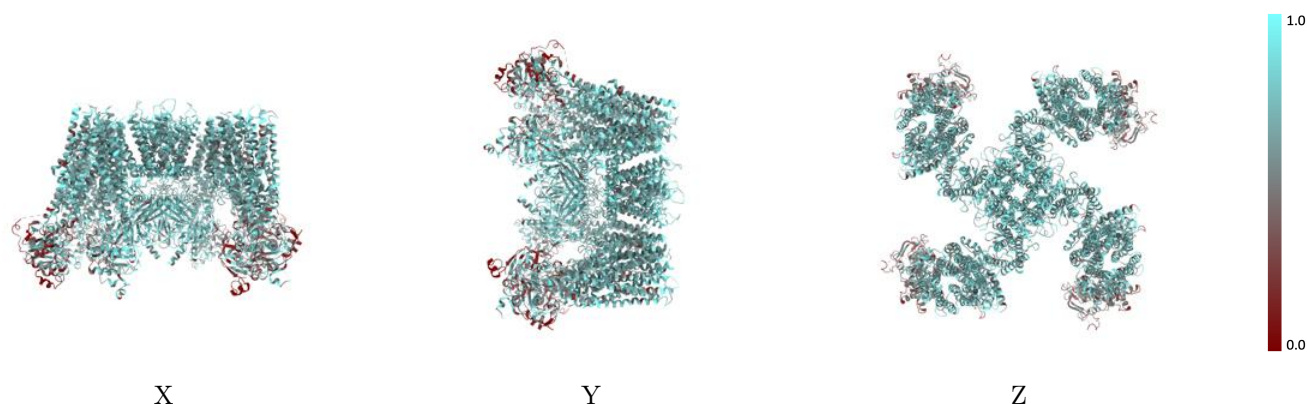
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



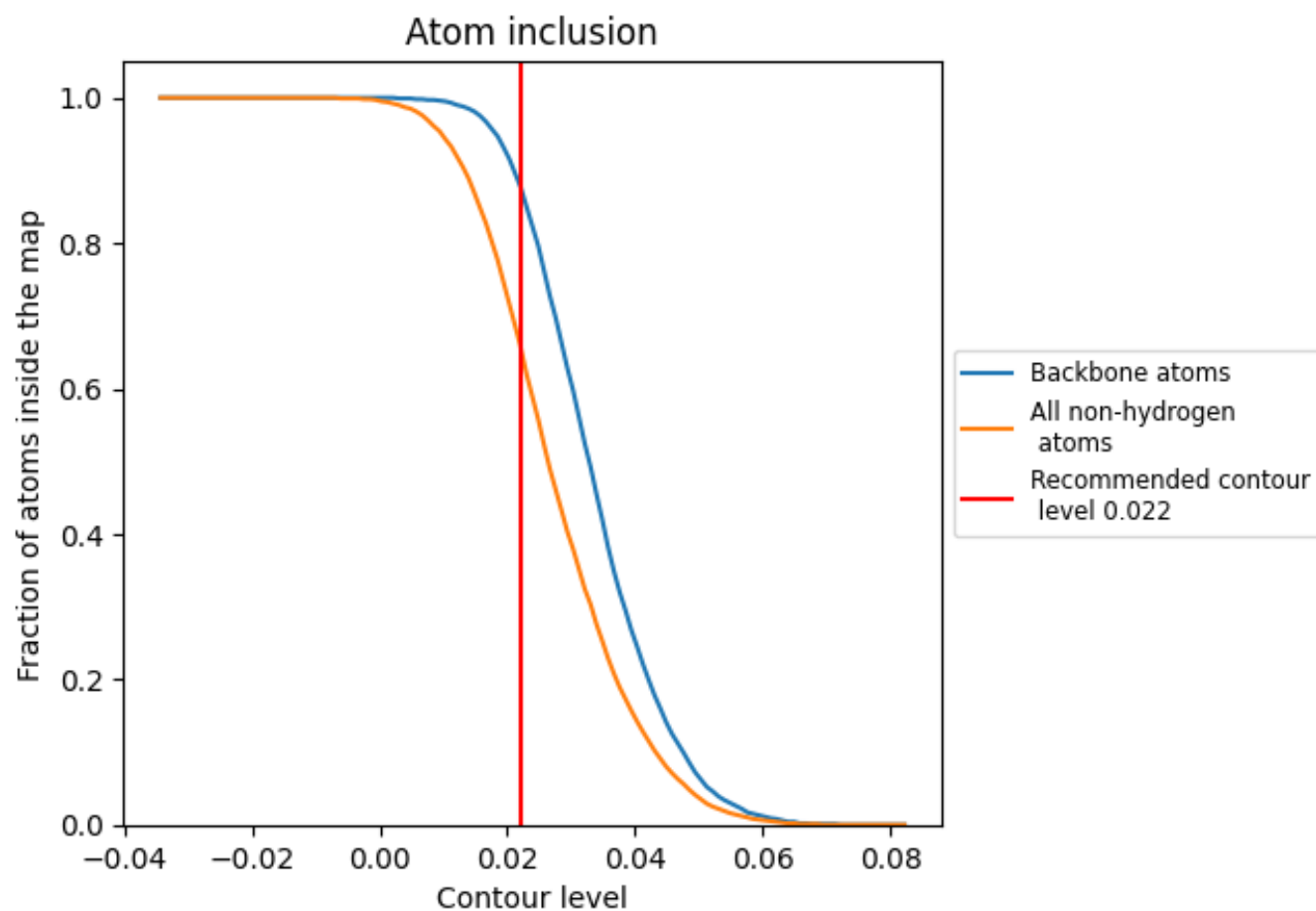
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6600	0.2260
A	0.7680	0.3100
B	0.6340	0.2050
C	0.7680	0.3090
D	0.6340	0.2060
E	0.7680	0.3100
F	0.6340	0.2070
G	0.7680	0.3100
H	0.6340	0.2070

